ABSTRACT BOOK

DSL2015 – Munich-Germany

22-26 JUNE, 2015

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PREFACE

It is our great pleasure to welcome you to the **11th INTERNATIONAL CONFERENCE ON DIFFUSION IN SOLIDS AND LIQUIDS: DSL2015** (Munich, Germany, from 22-26 June, 2015).

DSL-2015 aims at attracting a balanced portion of delegates from academia, industry and research institutions and laboratories involved with research and development work. In doing so, the conference provides a binding platform for academics and industrialists to network together, exchange ideas, provide new information and give new insights into overcoming the current challenges facing the academics and the industrialists relating to mass transfer, heat transfer, microstructure and properties, nanodiffusion and nanostructured materials.

I would like to thank the Organising Committee members and members of the Local Committee for their help in contributing to the successful organisation of this meeting and especially give thanks to Professor Stan Veprek for his support to help participants to get VISA's from the German Embassies.

I would also like to sincerely thank the organisers of the SPECIAL SESSIONS for their great work!

A special "thank you" as well to Professor Graeme Murch, Professor Ali Shokuhfar and Professor João Delgado, co-chairs of DSL-2015, for the excellent work, significant inputs and support to this conference.

You all made the way to Munich and I would like to personally thank you and all delegates for the decision to attend DSL 2015. I hope that you will find the meeting very useful for your work and business, as well as a useful forum for obtaining new knowledge.

Have fun learning and meeting new people!

See you again in 2016, in Split - Croatia!

12TH YEAR OF DSL!

Professor Andreas Öchsner
DSL CONFERENCES – Chairman

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Plenary Lectures:

VIP005
Prof. Stan Veprek
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Nanoscience and Nanotechnology: Why, When and How

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Why: Many properties of solids significantly change when the particle size decreases below 100 nm, and in particularly below 10 nm. I shall discuss the localization of surface plasmons, electronic quantum eigenstates and phonons as function of particle size and particle separation, and their effect on the properties of the nano-sized and nano–structured materials. It will be shown that not only the particle size, but also the particle separation plays an important role, because when the particle separation decreases below 1 nm, the electronic eigenstates begin to overlap and the confinement gets lost. Also the mechanical properties are significantly influenced by the particle size and their connectivity, and also by the scale of the experimental testing of conventional materials ("small is strong"). Nature has developed many nano-structured systems with hierarchic architecture, which provide unique mechanical and surface properties to plants and living species. For time limitations, I'll be able to bring only few examples from which we can learn a lot.

When a field suddenly becomes fashionable, it is essential to distinguish 'science facts' from 'science fiction'. I shall briefly mention some example where the 'nano does not work', and when one should better adhere to the conventional physics at the macro-scale.

How: The preparation of nano-sized and nano-structured materials requires special techniques which sometimes raises the question of the 'costs vs. gain'. The high dispersion (ratio of the number of the atoms at the surfaces to the atoms in the bulk) makes it difficult to keep nano-structured materials sufficiently pure, particularly free of oxygen impurities. For example, at an oxygen impurity concentration of 2-3 at.%, oxygen containing clusters in silicon decrease the diffusivity and the kinetically controlled crystallization, thus stabilizing amorphous silicon even at high temperatures of ≥ 600 °C. In nc-TiN/Si3N4 and related superhard nanocomposites, oxygen impurities of $\geq$ 1000 ppm (0.1 at. %) decrease the diffusion rate and segregation of the TiN and Si3N4 phases, thus apparently stabilize the TixSiyNz solid solution and hinder the formation of the stable and superhard nanostructure. The problem of impurities is not limited to oxygen only. For example it is known for more than 100 years that 100 ppm of bismuth in copper causes embrittlement of grain boundaries making copper very brittle metal. Yet, there is not any unambiguous, common agreement on the mechanism of that embrittlement. Obviously, there is a long way to go to understand all the important and relevant aspects of the nanoscience, and to learn how to utilize them in the technology, medicine and other fields.

VIP025
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Corrosion Behaviour of Equipment in High temperatures and Corrosion Resistant Alloys

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There are many damage patterns to high temperature corrosion which result from the fact that the materials are exposed to many kinds of environments and high temperatures.
Damage patterns can be roughly divided in two categories.
One is when the materials are damaged mainly by the effect of environment factors.

That is, when the materials are damaged by (1) high temperature oxidation, (2) steam oxidation, (3) molten salt corrosion, (4) high temperature particle erosion and erosion/corrosion, (5) high temperature sulfurization, (6) carburizing, (7) metal dusting, (8) nitriding, (9) high temperature chloride corrosion, (10) hydrogen attack, (11) liquid metal corrosion and so on.

The other is when the damages are caused by the degradation of characteristics of the materials themselves exposed at high temperatures.

That is, the materials are damaged through (12) thermal fatigue, (13) high temperature fatigue, (14) creep damage, (15) creep embrittlement, (16) sigma embrittlement, (17) 475 embrittlement, (18) tempering embrittlement, (19) graphitization and so on.

Phenomena and protective methods regarding the first category, damage caused by environmental factors, will be introduced using figures and tables mainly culled from my research.

Special Session 1
FLUID FLOW, ENERGY TRANSFER & DESIGN (SS1)

DSL096
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A New Mathematical Based Approach for Calculation of Diffusion Coefficient in Propagation of Fractal Signals

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Diffusion coefficient is a parameter which appears in mathematical equations that are related to fluid diffusion in different systems. Fractal system is one of the systems that can be modelled using diffusion equations. In this paper we develop a new formulation for diffusion coefficient in modelling of fractal signals' propagation. This equation is based on the equality of phase-lagging model of diffusion [1] and fractional diffusion equation. In fact, the governed diffusion coefficient has a relation with the Hurst exponent and time. The governed equation will be verified by considering the diffusivity in fractal systems. In order to do this task, we define dimensionless diffusivity as the ratio of governed time dependent diffusion coefficient to normal diffusion coefficient and then plot the dimensionless diffusivity versus the dimensionless temporal variable in three ranges of the Hurst exponent. The analysis of plots shows that as time goes on, the value of the dimensionless diffusivity increases, but after passing the maximum point, the dimensionless diffusivity shows the opposite behaviour and, after some time, the dimensionless diffusivity reaches a constant value. These results validate the mathematical approach and governed equation. Thus, by computing the value of diffusion coefficient at each time moment, and substituting its value in the fractional diffusion model the value of the fractal signal at each time moment can be computed with higher precision. The results of this modelling are useful not only in the modelling of fractal signals but can be applied in real time prediction of these signals.

[1] K. Seetharaman, H. Namazi, V. V.Kulish. Comput. Biol. Med., 42, 857 (2012).

DSL097
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Analysis of the Radius of Curvature in Two -Phase in Curved Pipeline with Leak

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The leak can present several manifestations characteristic signs, variation in pressure drop in position of leak, among other parameters. Techniques of leak detection available ranging from visual observation, to mathematical modeling through computational techniques [1].
There are many studies concerning flow in pipes, however most of these researches are experimental works. Given this situation, the CFD (Computational Fluid Dynamics) appeared as a tool to assist in understanding the

phenomena involved during fluid flow. Although there are papers in the area, the need exists for more research focused on thematic and especially leakage in ducts curved geometry (90 degrees).

This paper proposes numerical investigating the two-phase flow, a stream of oil containing water, in pipelines with curved in the presence of leaks via numerical simulation connections. The three-dimensional computational domain was created with the help of ANSYS CFX 12.1 commercial software package using complete equations of momentum and continuity equation. Eulerian-Eulerian model and the turbulence model SST (Shear Stress Transport) were adopted. The physical domain consists of a connection curve by 90 degrees which was varied the curvature radius. Numerical simulations in the study are isothermal and transient. Results of pressure and pressure drop for the simulated cases are presented and discussed. Results show influence radius of curvature on pressure drop the flow in the presence of leak.

[1] F.G. Aguiar, Neural networks for detection use in pipelines standards leaks. Master's thesis, São Paulo University, 2010.
[2] L.R.B. Sarmento., B.E. Leite., S.R. Farias Neto., A.G. Lima, Hydrodynamics of Oil-Water with Leakage by CFD, Defect and Diffusion Forum Vol. 348 (2014) pp 58-63.

DSL098
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Heat Transfer Analysis in a Ventilated Closed Cavity

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In this work, we propose a numerical study of the heat transfer in a square cavity with side of "H". The vertical walls are subjected to a temperature gradient $(\Delta T = T_h - T_c)$ while the horizontal walls are kept adiabatic. A volumetric fan, of diameter "D" and thickness "E", is placed in the middle axe of the cavity, and operates in the horizontal direction in order to ensure the cooling of the hot wall. This fan will create a pressure gradient "ΔP", modeled in our work, as a momentum generation in the Navier-Stokes equations.

The mathematical formulation of the problem is based on solving the continuity, momentum and energy equations. The dimensionless equations are made on the basis of reference parameters and finally appear controlling numbers (*i.e.* Rayleigh "*Ra*", Reynolds "*Re*" and the Rateau "*Rt*"). This last number gives the influence of the pressure gradient growth"ΔP". the finite volume method was used to discretize the obtained equations (and boundary conditions) and the resulting algebraic equations were solved by the SIMPLER algorithm.

The above figures illustrate the stream function lines "ψ" according to the different control parameters (*i.e. Ra*, *Re* and *Rt* numbers). Figure (a) shows the case where forced convection is predominant and the stream lines are represented by two principal cells $\left(\left|\psi_{max}\right| = 0.045\right)$. These two cells are symmetrical to the axis passing through the fan. Note that four small cells of low values have emerged in the cavity corners. When the Rayleigh number increases (see figure (b)) the contours of the stream function are in good agreement with those of conventional natural convection in the literature (Re<<Ra, pure natural convection).

In the next figure (Figure (c)) forced convection is more pronounced and dominant than the figure (a). A competition between natural and forced convection is obtained and the right two cells, controlled by the fan, cover the most part of the cavity. In the illustration (d, pour $Re=5\times10^{+2}$ et $Ra=10^{+6}$), we find that the contours of the two modes of convection (forced and natural) are coexisting in the cavity.
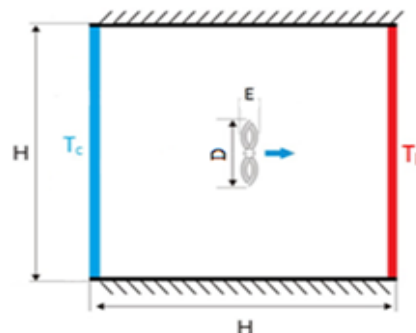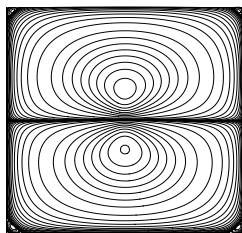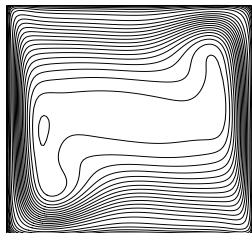
a : Re=10, Ra=1   **b** : Re=10, Ra=10^{+6} **c** : Re=5×10^{+2}, Ra=1   **d** : Re=5×10^{+2}, Ra=10^{+6}

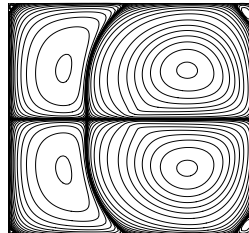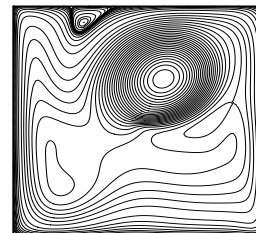Stream function for different values of the controlling parameters (Re, Ra et Rt =1).

Key words: natural Convection, forced Convection, mixed Convection, ventilated square cavity.

DSL100
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Theoretical Analysis and Simulation of Solar Pond Coupled with Heat Pipe

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The goal of this work presents the theoretical analysis at the heat extraction from solar pond by using heat pipe. The mathematical model used in this work is based on the heat conduction equation with external heat source. The source strength has been evaluated statistically over the period of the last five years according to the meteorology station data of Annaba "Les Salines". The problem solving approach of the mathematical model is based on the classical numerical methods taking on consideration heat loss of solar pond and it discredited scheme of the heat transfer equation with suitable initial and boundary conditions. For the heat pipe, a water loop was used for heating it. The aim of the present work is to determine the heat quantity extracted from the pond solar by heat pipe and changing some parameters like: number of heat pipes and the inclines of heat pipe

Key words:
Heat pipe, Heat transfer, Numerical modelisation

References:
[1] Dunn, P. D., Reay, D. A., 1994. Heat Pipes, fourth ed., Pergamon.
[2] Kays, W. M., London, A. L., 1994. Compact Heat Exchanger Design, third ed. Mc Graw Hill, New York.

DSL222
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Ejection and Cooling of Stainless Steel Film During Laser Cutting Process

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A purely analytical approach based on the boundary layer theory [1] has been developed to treat the laminar subsonic gas effects on the fusion laser cutting of stainless steel workpiece [2-4]. The purpose is to deduce the most efficient gas to blow out the molten metal from the formed kerf. Using nitrogen, argon and helium gas jets, the obtained results show that, when the shear stress and the velocity at the interface increase, leading to the increasing of the gas Reynolds number, the thickness of the molten boundary layer decreases along the kerf cutting edge. The argon and nitrogen are more efficient for cutting stainless steel than Helium gas. It has been also noted that helium allows a faster cooling and re-solidification of the molten layer. However, as it presents a lower shear stress, a bad cutting quality results, one can conclude that the helium should be not recommended for laser cutting of stainless steel. Moreover, the global resulting heat lost (conduction, radiation and convection) remains negligible compared to the incident laser power generally required for laser cutting. The obtained results show a good agreement with published works.

Keywords: cutting, laser, boundary layer, metal, gas, cooling.

References:
[1] B. S. Yilbas, Journal of Materials Processing Technology, 201, 285 (2008)
[2] M. Vicanek, G. Simon, J. Phys. D, 20, 1191(1987)
[3] C. Mas, R. Fabbro, Y. Gouedard, Journal of Laser Applications, 15, 145 (2003)
[4] A. Mahrle, E. Beyer, Proc. Of the Fifth Int. WLT-Conf. on Lasers in Manufacturing, LIM 215 (2009)
[5] H. Schlichting, Boundary Layer Theory, (McGraw-Hill, New York, 1982).

DSL242
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Analysis Oil-Water-Gas Three-Phase Flow in Curved Leak Pipe

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The production of oil and natural gas fields in onshore and offshore are characterized by the multiphase flow in ducts and pipes, and these are interconnected by various equipment such as wellhead, pumps, compressors, processing platforms, among others. The transport of oil and oil products is essential to the viability of the sector, with this movement oil is susceptible to fails, these faults causes great environmental damages and significant financial and image loss with society. Considering this necessity of the transportation sector of oil and derivatives, leakage in pipelines with curved connection, are object of study for various researchers [1,2,3]. In the sense, this work has a contribution the study of three-phase flow (oil-water-gas) in a curved pipe (90°) using the Computational Fluid Dynamics. The physical domain is constituted by two tubes of 4 meters trenched by a conector 90° curved, with the poring whole en the curveted accessory. The mathematical model is based on particle model, where is considered the oil as continuous phase and the water and gas as particulate phase. The turbulence model SST (Shear Stress Transport) was adopted. All simulations were carried out using the Ansys CFX® 12.1 commercial code. Results of the pressure, velocity and volumetric fraction of the phases are presented and discussed.

[1] A. Kalpakli, R. Örlü, Turbulent pipe flow downstream a 900 pipe bend with and without superimposed swirl, International Journal of Heat and Fluid Flow 41,103–111p, 2013.

[2] H. Mazhar, D. Ewing, J.S. Cotton, C.Y. Ching, Experimental investigation of mass transfer in 900 pipe bends using a dissolvable wall technique, International Journal of Heat and Mass Transfer 65, 280–288p, 2013.

[3] J. Marn, P. Ternik, Laminar flow of a shear thickening fluid in a 90◦ pipe bend, Fluid Dynamics Research 38, 295–312p, 2006.

DSL249
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Numerical Analysis of the Mixing Characteristics in Platelet Fluid Mixer

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Keywords: mixer, supercritical condition, platelet, hydrogen

Platelet mixer is a static mixer which can mix gases or liquids with different viscosity through platelet micro-channels cross-bedded injection technology. The structures of the platelet fluid mixer are very simple. It has no moving parts, and it can mix the fluid well in a very small chamber. In this work, the mixing process of gaseous and liquids hydrogen in the supercritical condition is considered. Firstly the structures of platelet fluid mixer are designed and the engineering estimations of pressure drop are conducted. Then the flow structures of platelet fluid mixer are numerically analyzed, Results indicated that the characteristics of the pressure drop are similar to the engineering estimations but the pressure drop is larger than other static mixer. The platelet fluid mixer can mix the fluid successfully on high pressure in a very small chamber which has no moving parts.

DSL271
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Analysis of Two-phase Pressure Drop Fluctuation Characteristics in a Single Mini-channel

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Two-phase pressure drop fluctuations during flow boiling in a single mini-channel were experimentally investigated. Degassed water was tested in circular cross section mini-channels with diameters of 1.0 mm, 1.6 mm and 2.0 mm at liquid mass fluxes of 21.19 kg m-2 s-1, 42.39 kg m-2 s-1 and 84.77 kg m-2 s-1 as well as heat fluxes of 0~216 kW m-2. Effects of heat flux, mass flux and channel diameter on pressure drop fluctuations were discussed based on the Fast Fourier Transformation results of the measured pressure drop and channel surface temperature. Three

basic types of fluctuations are identified, i.e. low-frequency fluctuation (~0.1Hz), medium-frequency fluctuation (~1Hz) and high-frequency fluctuation (~10Hz), the main causes of which were considered to be the alternation between liquid/two-phase/vapour flows[1-3], the process of bubble nucleation and growth[1-2] and the process of bubbles coalescence and collision respectively. A flow boiling map in terms of heat flux vs. mass flux is presented, showing the single-phase and two-phase regions. The two-phase region is subdivided into superimposed low-frequency low-amplitude fluctuation and medium-frequency low-amplitude fluctuation (LALF&LAMF) region, superimposed medium-frequency low-amplitude fluctuation and high-frequency low-amplitude fluctuation (LAMF&LAHF) region and low-frequency high-amplitude fluctuation (HALF) region. Besides, it is found that the LALF fluctuation is similar with the boiling onset oscillation[4] but with much shorter period and much lower amplitude. The LALF fluctuation is impeded with the increase of mass flux and channel diameter.

[1] Y. Wang, K. Sefiane, Z.G. Wang, et al., Int. J. Heat Mass Tran., 70, 353 (2014).
[2] D. Bogojevic, K. Sefiane, A.J. Walton, et al., Int. J. Heat Mass Tran., 30, 854 (2009).
[3] G. Hetsroni, A. Mosyak, E. Pogrebnyak, et al., Int. J. Mutiphas. Flow, 31, 371 (2005)
[4] Q. Wang, X.J. Chen, S. Kakac, et al., Int. J. Heat and Fluid Flow, 17, 418 (1996)

DSL277
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Development of Mathematical Models and Software for Launch Control Blast Furnaces

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Construction and development of automated process control systems on modern steel plants is characterized by the introduction and widespread use of computer decision support systems, which are based on mathematical modeling techniques.

The report examines issues the modeling processes occurring in the blast furnace during the first blow. Blowing in of blast furnace is a starting time of the blast furnace after the construction or major repairs, which starts with the deck after when a coke blast furnace and ends in the establishment in the furnace temperature field characteristic of a normally operating oven. All further long-term work of the blast furnace and the technical and economic performance of its work depend on the success of this operation.

The current approximate calculation methods blowing-in burden are based on the practice of blowing previously commissioned furnaces. Here we consider the direction theoretically little studied, there are no common evidence-based selection methods of the charge and blast parameters.

The most widely used two ways of blowing blast furnaces are the traditional and forced. The main difference is in the number and location loaded into the furnace charge. In the traditional blowing about 10 batches with a gradual increase of the ore load are charged up into the furnace. When forced method is used there is no need of gradually increasing load of ore and as a result less number of batches is required.

Currently, advanced metallurgical enterprises adhere to the concept of forced blowing, which speeds up the furnace operating parameters and reduces the risk of an accident. In the report this method is considered as the most promising.

Research methods used by the authors, are based on the physical laws of the basic processes occurring in the blast furnace, on the system analysis, on the use of modern design principles and construction of mathematical models, algorithms and software, which are designed for automated control of complex technological processes in metallurgy.

The following results are obtained by the authors:

1. A complex of mathematical models to calculate the location of the charge along the furnace height, choice of optimum blowing and gas-dynamic parameters was developed.
2. General principles of choice of blowing-in charge, blast and gas-dynamic parameters are formulated. The physical rationale and mathematical description of the limiting parameters of the blast furnace during blowing is given. Optimization model is created.
3. The software for engineering and technological staff of blast furnace was developed.

DSL278
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Numerical Simulation of Leakage of Oil in a Submerged Duct and the Behavior of Oil in a Marine Environment.

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The leakage in pipelines, beyond financial losses, can result in major environmental damage. In this way, the knowledge of interfacial phenomena of immiscible liquids allow us to understand the advective migration process in subsea pipelines. This information will enable predict the behavior and the geometric shape of water-oil interface and provide a good basis on perturbation theory, stability criteria, mathematical modeling and on the flow patterns in the vicinity of the leak in submerged pipelines [1,2]. The objective of this work is to study numerically the behavior of the leak in a submerged pipeline transporting oil. A two-dimensional mathematical model was used with a basis in the mass and momentum conservation equations and using the standard k-e turbulence model avaiable in Ansys CFX. A mesh with 40.510 hexaedral elements was used. The dynamic behavior of oil is introduced from the pressure field, by superficial velocity of the oil and by water volumetric fraction. Furthermore, an analysis about the results was made.

[1] A.B. Black, C.D. Grey and E.F. White, J. Appl.Phys., 50, 1234 (1990).
[2] S. Wang, in Focus on Multidimensional Microscopy, Vol.1, p.567, P.C. Cheng, Ed. (World Scientific, Singapore, 1999).

DSL279
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Numerical Evaluation of the Pressure Drop in the Multiphase Flow in Catenary Riser with Presence of Leakage

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The growing demand for oil brings the need for discovery of new reserves in deeper and deeper reservoirs, highlighted to ultra-deepwater. Thus, production in marine systems using components such as risers (flexible or rigid pipes) has been focus of many studies in different areas of knowledge. These ducts are used in transportation of multiphase fluids (oil, water and gas) produced from the oil well located on the seabed to the platform surface production. Due to the extreme conditions present in the offshore fields of production, the equipments that transport produced fluids operate close to their limits. So eventually, the flexible pipe structural may have integrity faults like leaks, which can cause production losses, accidents with victims and environmental disasters [1]. The leak depends of a number of properties or parameters measured at the site of the leak, for example, integrity of the pipe material, release of fluids and noise emission characteristic or manifestation of some other type of signal behavior, variation of pressure drop close to the leak, among others. There are a variety of techniques available for detecting leaks, among which there is the mathematical modeling using computational techniques [2]. In this context, this paper aims to study the fluid dynamics of a multiphase flow in transient regime in a catenary riser in the presence of a leakage. It was applied the equations of conservation of mass and linear moment and a model of turbulent flow (RNG k-ε), using the commercial package ANSYS CFX® to perform all simulations. The numerical results of velocity and pressure of the involved phases are presented and discussed.

[1] Y. Bai, Q. Bai, Subsea Pipeline and Risers, London: Elsevier Ocean Engineering Book Series, 1st edition, vol 1, (2005).
[2] L.M.C. Barbosa, A.G.B. Lima, S.R. Farias Neto, International Journal of Modeling and Simulation for the Petroleum Industry, 2, 23 (2012).

DSL288
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Wall Effects on Diffusion Coefficients in Nanochannel Flows

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Molecular Dynamics simulations are employed in order to investigate atomic flows in nanochannels, taking into account parameters such as wall/fluid interaction and roughness geometrical characteristics (shape, depth and length) which may not be important at the macroscale, but they are of significant importance at the nanoscale. From the atomic-scale analysis, we are able to derive transport properties such as the diffusion coefficients, which reveal the mechanisms of mass transfer and their calculation becomes valuable as experimental measures are difficult to perform at these scales.

One of the main implications considered in nanoflows is the finding, in both theoretical and experimental studies, that the classical hypothesis of the no-slip condition breaks down. Slip has been measured experimentally at small scales from the limit of 1mm [1], while it is shown that slip length reduces by periodic and random surface roughness compared to atomically smooth rigid walls [2]. As a result, diffusion coefficient values are also affected by wall characteristics [3] and their behavior seems to be connected somehow with the calculated slip length values [4].

In this work, we study the combined effect of nanochannel design properties such as wall roughness shape, depth and length, along with the wall wettability properties (hydrophobic or hydrophilic wall), on the calculation of nanochannel diffusion coefficients. We believe that our calculations could serve as a guide to reveal all possible implications that could arise during theoretical and practical nanochannel design.

[1] D.C. Tretheway and C. D. Meinhart, Phys. Fluids 14, L9 (2002).
[2] N.V. Priezjev, J. Chem. Phys. 127, 144708 (2007).
[3] W.P. Krekelberg, V.K. Shen, J.R. Errington, T.M. Truskett, J. Chem. Phys. 135, 154502 (2011)
[4] F. Sofos, T.E. Karakasidis, and A. Liakopoulos, Heat Mass Transf. 49, 1081 (2013).

DSL342
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3D Simulation of Micron Size Particles Movement in an Acoustic Pressure Field
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In this article a 3D simulation method based on finite element method is introduced to evaluate particles behaviour in an acoustic pressure field. Manipulation of micron size particles using acoustic force are progressing in recent years. Particles in fluid flow excited by the acoustic pressure field inside the microchannel, experience acoustic force, drag force, buoyancy and gravity force. Among these forces, buoyancy and gravity force are balanced in the middle parts of the channel. So, we focus on acoustic and drag forces effect on particles displacement in fluid flow. The acoustic force on microparticles is proportional to some factors like size, density and compressibility while drag force is proportional to the radius of the microparticles [1],[2]. A numerical method is used for modeling fluid flow in a microchannel and calculating acoustic force varying with time on two special microparticles. Piezoelectric , pressure acoustic and particle tracing modules, used for simulating. Comsol multiphysics 4.3b, is a finite element software to model multiphysics problems. Acoustic pressure field modeled by acoustic pressure module (acpr) , fluid domain modeled by laminar flow module (fpt) and the positions of particles inside the microchannel modeled by particle tracing for fluid flow physic (fpt). By following the particle direction, we will find out how acoustic force and drag force affect particle movement.

[1] Y.K.K. Yosioka, Acoustic radiation pressure on a compressible sphere, Acustica 5 (1955) 167–173.
[2] J.J. Shi, H. Huang, Z. Stratton, Y.P. Huang, T.J. Huang, Lab on a Chip 9 (2009) 3354–3359.

DSL399
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Operating Activity Visualization and Thermal Performance Measurement of Pulsating Heat Pipe
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Heat pipe is well known device which is used to heat transfer phase-change of working fluid. Pulsating heat pipe (PHP) is special type of heat pipe which heat transfer by pulsating movement of working fluid. Article deals about operating activity and thermal performance measurement of this special heat pipe. Operating activity visualization of PHP was performed with PHP made from glass. The two types of PHPs were made. The first PHP has internal diameter of pipe 1 mm, second PHP has internal diameter of pipe 1.5 mm and both PHPs have eleven meanders. The working fluids used in PHP were water and Fluorinert FC-72. These fluids were chose for their different

thermo-physical properties and the visualization observe formation of liquid and vapour phase working fluid during filling process and working operation. Next, the article describes thermal performance measurement of PHP depending on working fluid amount and heat source temperature. Measurement was performed with PHP made from copper pipe with inner diameter 1.5 mm curved to the twenty one meanders and filled with water. The results give us image about formation and distribution of working fluid in pulsating heat pipe and about influence of working fluid amount on the heat transfer ability of pulsating heat pipe.

DSL401
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Numerical Simulation of Double Pipe Heat Exchanger Inserted with Twisted Tape with Film Condensation of Water Vapor

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In this work an numerical study on turbulent flow with film condensation of water vapor through a horizontal double pipe heat exchanger with and without twisted tape are presented. The effect of inserting twisted tape and his geometric characteristics such as twist ratio on the average heat transfer coefficient and pressure loss in the Reynolds number range from 5,000 to 12,000 are investigated. Outer flow of condensing water vapor releases heat to the cold inner flow of water in counter flow heat exchanger. At first the numerical results are compared with experimental work and the agreement between them, with and without twisted tape, are found to be satisfactory. The numerical results reveal that heat transfer coefficient and friction factor in inner pipe equipped with twisted tape, are higher than those without twisted tape. It is also found that both heat transfer coefficient and friction factor increased by using twisted tape dramatically. For comparison, the variation for Nusselt number and pressure loss is about 8%. By increasing the twist ratios the amount of pressure loss, heat transfer coefficient and the film condensation rate through pipe is decreasing. In addition, the value of thermal performance factor ( ) for double pipe with and without twisted tape is also presented. The influences of film condensations in both of them are determined. By increasing Reynolds number the amount of turbulence intensity goes up and the effect of twisted tape has showed better.

Keywords: Film Condensation, Heat Exchanger, Twisted Tape, Turbulence Flow, Pressure Loss, Nusselt number.

DSL408
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Misaligned Porous Journal Bearings Lubrication Analysis by Including the Thermal Effects

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It is well known in conventional journal bearing lubrication studies, the thermo-hydrodynamic aspect analysis is focused essentially on the aligned journal bearings by neglecting the rotating shaft deflection [1-2]. However, they are the main causes of premature wear of these mechanisms. According to the literature review, under isothermal boundary conditions assumptions, extensive works have been reported to determine the characteristics of misaligned rigid journal bearings [3-4]. El -Butch et al. [5] noticed that the increase in journal misalignment deteriorates the oil film thickness and leads to the wear metal- metal contact issue. In the present work, a numerical study of the effect of misaligned porous journal bearing caused by shaft deformation is analyzed by taking into account the thermo-hydrodynamic lubrication aspect. The generalized Reynolds equation is derived according to thermal aspect, the porous structure and the shaft misalignment degrees, where the Darcy's law is used to determine the fluid flow through the porous matrix. The heat transfer equation and the Reynolds equation are numerically solved by used the finite difference method.   Different parameters are calculated versus the misalignment degree, the eccentricity ratio and the porous bearing permeability. The results obtained in this study have compared with those of the literature, where a good agreement is observed.

[1] S. Boubendir, S. Larbi, R. Bennacer. Tribology international, 44, p. 1-8 (2011)
[2] S. Boubendir, S. Larbi, R. Bennacer. D.D.F, 297-301, p. 618-623 (2010)
[3] J. Sun, G. Changlin. Tribology international, 37, p. 841-848 (2004)
[4] S. Das, S. K. Guha, A. K. Chattopadhyay. Tribology international, 35, p. 201-210 (2002)
[5] A.M. El-Butch, N.M. Ashour. Tribology International, 38, p. 41–48 (2005)

VIP064
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Optimization of Sensible Thermal Storage Systems by Genetic Algorithm and Generalized Extremal Optimization

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The present paper presents some aspects of the optimization of a sensible thermal storage system based on a lumped approach. The thermal system is composed by parallel flat plates and the a energy transport fluid (air). The flat plates are modelled as lumped volumes and air is taken as non-capacitive. The main parameters that describe the behavior of this system are the plates geometry, its material properties and the flow rate of the working fluid.

These parameters are optimized by both a stochastic algorithm called the Generalized Extremal Optimization (GEO) and a Genetic Algorithm (GA. The objective function is to find the lowest difference between the air outlet temperature and the a reference temperature. The GEO method delivers results about 50 times faster, with the same numerical quality.

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VIP066
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Numerical Study of Turbulent Forced Convective Jet Flows Employing Different Closure Models

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The present work exhibits a numerical study of turbulent jet flow in cylindrical cavity with convective heat transfer employing different methods to tackle with turbulence for prediction of time-averaged and statistical fields of these kind of flow. More precisely, four different approaches for treatment of turbulence are employed: Large Eddy Simulation (LES) with dynamical Smagorinsky subgrid model (DSSGS), k - e, k - w and RSM (Reynolds Stress Model), which are based on the Reynolds-Averaged Navier Stokes (RANS) framework. The conservation equations of mass, momentum and energy are solved with the Finite Volume Method (FVM). All simulations are performed for a turbulent jet (free turbulent shear flow) with ReD = 22000 and Pr = 0.71. In the forced convective subject, the main purpose is to verify if the employment of different turbulence closure models can led to reasonable differences in the thermal fields and convective fluxes on the cavity surfaces. Differences for predictions of time-averaged and statistical fields are also important for future analysis of turbulent flows with combined convective and radiative transfer in participant media, i.e., investigating the influence of Turbulent Radiation-Interactions (TRI). Results revealed that the jet flow has a higher penetration into the cylindrical cavity for the simulation performed with LES, while a higher radial scaterring is seen for the simulations with RANS. In spite of similar tendency, large discrepancies are noticed for the time-averaged, statistics and convective fluxes predicted with LES and RANS. These discrepancies led to different predictions of turbulent flows with combined convective and radiative transfer, even in non-reactive flows where TRI is considered negligible.

Keywords: LES, RANS, turbulence, cylindrical cavity flows.

DSL203
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Numerical Simulation of Flow Two-Phase (oil-water) no Isothermal in the Presence of Leak in Curved Connections

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The transport of oil and its derivatives have been done in the large majority through pipeline networks linking the oil fields, refineries and distribution networks for consumer centers. And this has been the best way of transportation of oil, especially in Pipelines are widely used in the chemical and petrochemical industries for transporting fluids. Leaks of hazards fluids such as crude oil and gasoline can result in very serious environmental pollution if the leak is not quickly detected and repaired. Leaks can cause loss of life, environmental cleanup costs, possible fines and legal suits, for example [1-2].

What stimulates the development of reliable techniques for the rapid and accurate detection of leaks along the pipeline in order to eliminate or minimize the loss and environmental damage. Understanding the flow behavior in the presence of leakage enables indication of the effective techniques for leakage, avoiding the generation of false alarms. This study evaluated the effect of numerically presence of leakage of the two-phase flow (oil-water) in the pipeline connections using commercial software ANSYS CFX. With the field of volume fraction, temperature and velocity and pressure profiles, it was possible to evaluate the influence of leakage flow and the evolution of

pressure and pressure drop with time. The results from the fields of pressure, velocity and volumetric flow rate are presented and assessed for illustrating the effect of the presence of the leak in the dynamics of flow in curved pipe.

[1] Barbosa, L. M. C.; Lima, A. G. B.; Farias Neto, S. R.(2012). Non-Isothermal Transient Three-Phase Flow (Heavy Oil, Water and Gas) in Vertical Pipeline: The Effect of Leakage. International Journal of Modeling and Simulation for the Petroleum Industry, 6(2), p. 23-31.
[2] C. Green, Multi-leak detection and isolation in fluid pipelines, Control Engineering Practice Journal, Vol. 9, pp. 651-682, (2001).

DSL235
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Numerical Simulation of Thermofluidynamics of Pollutants Dispersion in a Thermoelectric

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The growing global demand for energy has led researchers to seek the improvement of technologies, in order to maximize the generation of electricity in its different forms. Among the different methods of production is the energy produced by thermal power plants, which account for more 60% of the energy produced in the world [1]. This is a form of energy generated from the combustion of fuels such as coal, diesel oil, natural gas and others. Among the main problems caused by the production of thermal energy is the emission of gaseous pollutants to atmosphere, such as carbon dioxide (CO_2), sulfur dioxide (SO_2), nitrogen oxides (NO_x), and also particulate matter which cause environmental problems such as acid rain, greenhouse effect, and health problems, especially respiratory [2].

Computational fluid dynamics (CFD) is presented as a most important tool in solving problems involving dispersion of chemical species to the atmosphere. In this sense, this study aims to evaluate the thermofluidynamics of pollutants dispersion emitted from the chimney of a thermal power plant, based on numerical simulations in the Ansys CFX 12.0 commercial code, using a transient non-isothermal model, under different conditions of atmospheric stability. Fields of pressure, velocity, temperature and mass concentration of the different components involved in the process are presented and analyzed.

[1] U.S. Energy Information Administration / Monthly Energy Review November (2014).
[2] L. Z. D. VILLANUEVA, Reducing the impact of air pollution in power plants. Case study: thermal power plant Iquitos, Master's thesis, Postgraduate in Energy, USP, São Paulo-SP (1998).

DSL247
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Novel Diffusimeter for Turbulent Super Diffusion of Electrolytes with Relative Rates Proportional to Respective
Molar Mass Square Root

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The U-tube like diffusimeter with straightway stopcock at each end lets MCl(aq) (M = H, Li, Na, K, and Rb) and AgNO3(aq) reactant pairs diffuse towards each other through water to produce white AgCl(s) as indicator at the intersection. High concentration gradient at each solution-solvent interface of the diffusimeter generates mild, turbulent diffusion-convection that gives rise to super diffusion with rates about 102 times higher than normal liquid diffusion and an apparent rate law, V∞√M contradicting V∞√(1/M) for gases. The heavier electrolyte in the diffusimeter travels faster. Distance travelled ratio (DTR) of a reactant pair and their molar mass ratio square root (MMRSR) taken in order are closely equal. Rate versus concentration plots for MCl-AgNO3 follow Fickian trend. The MCl and AgNO3 do not show to carry any coordinated H2O.

Keywords: Convection, Turbulent diffusion, Mass transfer, Diffusimeter.
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DSL318
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HF Diffusion Coefficients in Polymers used for Microelectronic Applications

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Since mid 1990's, polymers are used as materials of construction for Front Opening Unified Pods (FOUPs) which are used throughout the microchip manufacturing process to protect and transport environmentally sensitive silicon wafers on which IC chips are made. Some IC chip manufacturing process steps require the use of corrosive halogenated gases for etching. Residual ppb levels remaining on process wafers stored inside the FOUP outgas into the clean FOUP environment where they are absorbed by the FOUP polymers and later desorbed in a subsequent process step causing corrosion to sensitive metal layers and yield loss. We have studied this sorption and outgassing mechanism in relation to FOUP environment control employing different polymers and have reported on it previously [1]. In order to understand our findings we have measured different FOUP polymer's transport coefficients. As sorption is governed by surface adsorption of molecules then, followed by their diffusion into the polymer bulk, diffusion via outgassing becomes the key parameter to understand cross contamination mechanisms. In this work, we present the transport coefficients obtained for gaseous HF at cleanroom conditions (Patm, 25°C & 40% RH) for sorption and desorption processes; using the steady state method, based on Fick's first law in thin films polymers (<80μm) that constitute FOUPs (i.e. Polycarbonate, Polyetherimide and a low absorbing material named Entegris Barrier Material EBM). Results show low HF Diffusion coefficients (between 3.7E-12 and 17E-11cm²/s).

[1] P. González-Aguirre, H. Fontaine, C. Beitia, J. Ohlsen, J. Lundgren, P. Lee. A comparative study of the HF sorption and outgassing ability of different Entegris FOUP platforms and materials. Microelectronic Engineering, 105 (2013), 113-188

DSL322
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Unsteady Laminar Mixed Convection Heat Transfer from two Horizontal Confined Isothermal Cylinders in Tandem

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Detailed numerical simulations are carried out for transient mixed convection in a laminar cross-flow from two isothermal cylinders in tandem arrangement confined inside a vertical channel. Using the vorticity-stream function formulation of the unsteady two-dimensional Navier-Stokes and energy equations, the governing equations are solved numerically using the control volume method [1] on a non-uniform orthogonal Cartesian grid. Simulations are performed for fixed values of the geometrical parameters, Reynolds number based on cylinder diameter of Re = 200, Prandtl number of Pr = 0.774, blockage ratio of D/H = 0.3, and a pitch-to-diameter ratio of L/D = 2. Results illustrate the effects of buoyancy strength or Richardson number Ri = Gr/Re2 on the overall flow structure and nondimensional heat flux (Nusselt number) from the cylinders. The results reported herein demonstrate how the flow structure and heat transfer characteristics of the cylinder array are affected by the wall confinement [2] and interference effects.

[1] J. Marroquín-Desentis, C. Treviño, J.C. Cajas, E. Salcedo and L. Martínez-Suástegui, Int. J. Heat Mass Transfer, 84, 766 (2015).
[2] I. Guillén, C. Treviño and L. Martínez-Suástegui, Exp. Therm. Fluid Sci., 52, 30 (2014).

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Three-Dimensional Buoyancy Effects for Transient Laminar Opposing Mixed Convection Heat Transfer from two Heaters in a Duct Preceded with a Plane Symmetric Sudden Contraction-Expansion

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An experimental investigation of laminar opposing mixed convection is carried out to assess the effect of opposing buoyancy in an open vertical rectangular channel with two discrete protruded heat sources subjected to uniform heat flux simulating electronic components. Experiments are performed for a Reynolds number of Re = 300, Prandtl number of Pr = 7, channel inclination angles with respect to the horizontal of γ = 0o, 45o and 90o, and different values of buoyancy strength or modified Richardson number, Ri* = Gr*/Re2. The time evolution of the temperature distributions along the discrete heat sources has been obtained, and the temperature measurements show that for relatively large values of buoyancy strength, strong three-dimensional (3D) secondary flow oscillations develop in the axial and spanwise directions. The results reported herein demonstrate how the time-dependent heat transfer characteristics at each protruded heat source are affected by the 3D configuration of the vortical structure that develops upstream and downstream of the partial blockage.

DSL336
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Buoyancy-Driven Heat Transfer in a Finned Cavity Filled with Nanofluids

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The natural convection in a square cavity with differentially-heated vertical walls and insulated horizontal walls filled with nanofluids is investigated numerically. A horizontal, perfectly conducting, thin fin is attached to the left vertical wall of the cavity. The left vertical wall and the fin are maintained at a temperature higher than that of the right side-wall. Two different nanofluids, namely, Cu-water and Al2o3-water are utilized in this study. The governing equations written in terms of the primitive variables are solved numerically using the finite volume method and the SIMPLER algorithm. Using the developed code, a parametric study is performed and the effects of the length and position of the fin, the volume fraction of the nanofluids and the Rayleigh number on the fluid flow and heat transfer inside the cavity are investigated. The results show heat transfer enhancement with increasing the volume fraction of nanoparticles.

DSL352
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Thermal and Stress Analyses of Ring Core Doped Double Clad Fiber

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We formulated, studied and analyzed the thermal and stress properties of a proposed ring core Ytterbium doped double clad fiber. The analysis has shown that the ring core doped fiber gives an improvement in the temperature and stress profiles as compared to the conventional core doped double clad fiber with similar effective doped area. This is promising for the high power fiber laser where the thermal effects must be managed properly to ensure good system efficiency. The thermal and stress handling capability can be further improved by changing the ring core doped position as well as the doped thickness. It has been found out that the further the doped position, the better the thermal behaviour, i.e. lower core temperature.

We begin by solving the heat diffusion equation for the three different regions within a ring core doped double clad optical fiber, namely undoped core, doped core and cladding regions. This leads to explicit expressions for the radial thermal distributions, radial stress, tangential stress and z- stress profiles in the mentioned regions. The regions are assumed to have similar thermal and mechanical properties as they are made of the similar glass materials.

Having understood the thermal and stress behaviours of the ring core doped double clad fiber in fiber lasers, we then studied the power scaling capabilities of the mentioned fiber. We found that the fiber can give very good improvement in the high power scaling capabilities. Six parameters are studied to determine the limitation of the power scaling, namely thermal fracture, core melting, thermal lensing, optical damage limit, pump brightness as well as nonlinear effects (i.e. Stimulated Raman Scattering for broad band case and Stimulated Brillouin Scattering for narrow band case).

VIP024
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Why does Some Biological Networks Deviate from Hess-Murray Law and why is this Question of Importance?

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Complex flow systems such as the vascular and respiratory trees are made of large and small vessels in series. This compromise between large and small vessels is due to the fact that systems involve both translational and transmural flows. The optimal arrangement of vessels in these tree-networks seems to obey to Hess-Murray law, which pointed out a relationship that links the radius of a parent vessel (immediately upstream from a vessel bifurcation) to the radii of the daughter (immediately downstream after a vessel bifurcation): the reduction of vessel size by a constant factor ($2^{-1/3}$). However, there are some experimental evidences that there are tree-networks that present larger sizes than predicted by the Hess-Murray law (e.g. the acinar airways of the respiratory tree). How and why is this possible? Is the maximum physical efficiency, in some cases, not a sufficient criterion for the physiological design?

In this study we describe the fluid flow through several tree-networks arrangement based on constructal law. We show that the physical optimization (maximal flow access) in the tree-network design is not always given by a reduction of vessel size by a constant factor of $2^{-1/3}$.

VIP026
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Geometric Study of Highly Conductive Materials Applied to Cooling by Heat Conduction

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This work proposes the use of "Constructal Design" method to perform the study of the effect of geometry on the performance of a system in form of "V" that removes constant heat flux of a body through isothermal heat sinks. The equation of heat conduction in steady state, using constant properties, is applied to the system of interest. It will be numerically shown that the overall thermal resistance of the path in "V", subject to constant total area with the form of a circle, as well as constant V-shaped conductive pathway area, can be minimized by varying the V-shaped geometry (degrees of freedom). The results show that "Constructal design" method leads to an emergence of a V-shaped conductive pathway configuration which improves the performance of the system.

Keywords: constructal design, heat conduction, V-shaped conductive pathways.

VIP035
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Drying Characteristics of Fine-Particle Lignite in Paddle Dryers

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Drying is an important way to improve the quality of lignite with high moisture. In this paper, a single-shaft paddle dryer experimental system was built to investigate the drying characteristics of fine-particle lignite with diameter 0-5mm. The experimental results show that with the increasing in shaft rotation speed the flow rate of lignite increases linearly approximately and the residence time decreases correspondingly. Increasing the inclination angle helps increase the flow rate. Both shaft rotation speed and heating source (heat transfer oil) temperature have significant effects on outlet moisture content of lignite. Shaft rotation speed affects the average heat transfer coefficient greatly and heating source affects it weakly. It is found that for 5-12mm coarse-particle lignite, flow is not smooth and the average heat transfer coefficient is much less than that of fine-particle lignite. This research shows that it is feasible technically to dry fine-particle lignite using paddle dryer, which is not suitable for drying coarse-particle lignite.

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Dissipation Effect on Forced Convection in Triangular Cross Section Microchannels with Nanofluids

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Heat transfer of fluids is very important to many industrial heating or cooling equipments. Convective heat transfer can be enhanced passively by changing flow geometry, boundary conditions or by enhancing the thermal conductivity of the working fluid. An innovative way of improving the thermal conductivity of base fluids is to introduce suspended small solid nanoparticles. In this paper a numerical investigation on laminar forced convection flow of a water–Al2O3 nanofluid in a triangular microchannel is accomplished taking into account the dissipation. A constant and uniform heat flux on the external surfaces has been applied and a single-phase model approach has been employed. The analysis has been performed in steady state regime for particle size in nanofluids equal to 38 nm.

The base fluid is water and nanoparticles are made up of alumina (Al2O3). The length the edge and height of the duct are 0.030 m, 1.7 x10-7 and 1.1 x10-7 m, respectively. In this way, the hydraulic diameter is set equal to 8.3x10-7 m. Results are presented in terms of temperature and velocity distributions, surface shear stress and heat transfer convective coefficient, Nusselt number and required pumping power profiles. Comparison with results related to the fluid dynamic and thermal behaviors are carried out in order to evaluate the enhancement due to the presence of nanoparticles in terms of volumetric concentration.

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Theoretical and Numerical Optimisation of Conjugate Heat Transfer of Different Cross-Sectional Shapes with Internal Heat Generation:
A Review

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In this work the cooling channels of five different cross-sectional shapes were studied: Circular, square, rectangular, isosceles right triangle and equilateral triangle. They were uniformly packed and arranged to form a larger constructs. The theoretical analysis is presented and developed using the intersection of asymptotes method to provide the existence of an optimal geometry of parallel channels of different cross-sectional shapes that penetrate and cool a volume with uniformly distributed internal heat generation and heat flux which minimises the global thermal resistance. Also, a three-dimensional finite volume based numerical model was used to analyse the heat transfer characteristics of various cooling channels cross-sectional shapes. The numerical computational fluid dynamics code has recently provided a more cost-effective and less time-consuming means of achieving the same objective. In this work a mathematical optimisation algorithm coupled with numerical computational fluid dynamics code is employed and incorporated into the finite volume solver- FLUENT and grid (geometry and mesh) generation package GAMBIT to search and identify the optimal design variables at which the system will perform optimally for more efficient and better accuracy. The algorithm is also specifically designed to handle constraint problems where the objective and constraint functions are expensive to evaluate. This automated process is applied to different design cases of cooling channels shapes. These cooling channels are embedded in a highly conductive solid and the peak temperature is minimised. The trend and performance of all the cooling channels shapes cases studied are compared analytically and numerically. It is concluded that optimal design can be achieved with a combination of computational fluid dynamics code and mathematical optimisation.

Keywords: Geometric configurations, computational fluid dynamics, mathematical optimisation, thermal conductivity, constraints, laminar flow, forced convection, optimal geometry, peak temperature, constructal theory, thermal resistance, Dynamic-Q,

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HYDROGEN-RELATED KINETICS IN MATERIALS (SS10)

DSL250
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Experimental Determination of the Critical Protective Cathodic Potential of API 5CT P110 Steel to Minimize the Risk of Hydrogen Embrittlement
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The corrosion control on metallic structures used in the offshore oil and gas industry is critical. Cathodic protection is one of the most reliable techniques used against corrosion in structural steels exposed to seawater. According standards of current use [1], a cathodic protection system is considered safe, whether the potential is in the range of -900 mVAg/AgCl to -1100 mVAg/AgCl. However, the upper limit is not applicable for steels with yield strength greater than 550 MPa, given that overprotection conditions can be generated in less negative potentials. In this conditions, large amounts of hydrogen can be produced on coating defects, which when absorbed into the steel can cause Hydrogen Embrittlement - HE. Thus, the knowledge of the upper limit, or "critical protective cathodic potential", is vitally important to minimize the risk of HE. This paper presents experimental data of HE susceptibility of API 5CT P110 steel on different cathodic potentials, as well as the minimum protective potential from which their susceptibility begins to grow. Samples for electrochemical and mechanical tests were extracted from pipe of P110 steel in the as-received conditions. Hydrogen permeation tests were performed at room temperature using a Devanathan-Stachurski electrochemical cell [2]. The apparent and effective diffusivity were calculated based on the elapsed time (tlag) from two consecutives hydrogen permeation curves plotted for each sample, and determined the minimum time to fully saturate the round tensile samples. These specimens, without and with hydrogen, were subjected to uniaxial tensile tests until fracture at room temperature, and HE susceptibility was evaluated. The results show that the API 5CT P110 steel has a high susceptibility to HE, and that the Critical Protective Potential to avoid overprotection and minimize HE is -900 mVAg/AgCl. Therefore, the recommended potentials by current technical standards are not applicable to studied steel.

[1] ISO 15589-2, Petroleum and Natural Gas Industries - Cathodic Protection of Pipeline Transportation Systems, Switzerland (2004).
[2] M.A.V. Devanathan and Z. Stachurski, Proceedings of the Royal Society, A270, 90 (1962).

DSL306
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Overpotentials Application of Cathodic Protection and its Harmful Effects on API 5L X65 and API 5L X70 Steels Due Hydrogen Permeation
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The use of cathodic protection to preventing the alloys corrosion and steels, is mainly due to their effectiveness in prolonging the structural and chemical integrity of these materials, promoting the increasing their useful life in corrosive environments. This technique is applied using sacrificial anodes (galvanic protection) or by direct printing current (impressed current protection).The structures commonly protected by this technique are pipelines, ships' hulls, storage tank, harbour structures and offshore platforms. However it is necessary some care and precautions in the application of this technique. The use of excessive negative potentials can cause other kind of problems due to hydrogen evolution on the metal surface resulting in hydrogen embrittlement especially in high strength steels

and low carbon alloys [1,2]. To contribute with the knowledges about the harmful effects of this phenomenon, it was studied in the present work the influence of the overpotential of cathodic protection applied on API 5L X65 and X70 steels submited to the assisted corrosion by hydrogen. Therefore, transients of permeation were obtained for different potentials (-1100 mV and -1300 mV vs. SCE). Measurement of diffusivity, permeability and solubility was estimated at temperature room (25±1ºC). For the overpotential of -1100 mV the permeation transients displayed the normal diffusion behavior, by the other hand, to the potential of -1300 mV, the permeation transients were displayed with anomalous behaviors for both steels, proving a phenomenon previously reported by Bockris and Subramanyan [3], for Armco iron and iron-nickel alloy (membranes of 5% Ni, 95% Fe) and by Beck et al. [4] for the same steel.

[1] BS EN 13173. Cathodic protection for steel offshore floating structure. 2001.
[2] International Standard ISO 12473. General principles of cathodic protection in sea water. 2006.
[3] J.O'M. Bockris, P.K. Subramanyan. Hydrogen embrittlement and hydrogen traps. J. Electrochem. Soc. Electrochemical Science., 118, 1114-1119 (1971).
[4] W. Beck, J.O'M. Bockris, J. McBreen, L. Nanis. Hydrogen permeation in metals as a function of stress, temperature and dissolved hydrogen concentration. Proc. R. Soc. Lond. A., 290, 220-235 (1966).

DSL307
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Evaluate of Mathematical Models Applied to Determine Parameters of Hydrogen Trapping Sites in Steels and Alloys

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Over the past several decades, have been proposed numerous mathematical models for investigating the phenomenon of hydrogen trapping in metals through parameters Eb (hydrogen trap binding energy) and NT (density of trap sites). However, in recent published works, mathematical models that have been used to determine NT and Eb contain errors or have been based on the work of researchers whose works contain no mention of equations or mathematical terms related to hydrogen trapping, which calls into doubt the validity of the models applicability. Given the previously discussed problems, the objective of this study was to review, identify and correct the faults present in some mathematical models used in the study of hydrogen trapping [1 – 6] and to show how these failures can affect the analysis and determination of the density of hydrogen trapping sites. To prove such failures, we performed electrochemical permeation tests on API 5L X65 steel to determine the apparent and effective diffusivity of hydrogen and the concentration of subsurface sites to determine the density of hydrogen trapping sites. In this work, based on permeation test results for X65 steel, we show that the use of incorrect mathematical models leads to values of NT that differ by four orders of magnitude.

[1] Yen SK, Huang IB. Critical hydrogen concentration for hydrogen induced blistering on AISI 430 stainless steel. Mater Chem Phys. 2003; 80: 662-6.
[2] Dong CF, Li XG, Liu ZY, Zhang YR. Hydrogen induced cracking and healing behavior of X70 steel. J. Alloy Compd. 2009; 484: 966-72.
[3] Dong CF, Liu ZY, Li XG, Cheng YF. Effects of hydrogen charging on the susceptibility of X100 pipeline steel to hydrogen induced cracking. Int. J. Hydrogen Energy. 2009; 34: 9879-84.
[3] Hadžipašić AB, Malina J, Malina M. The influence of microstructure on hydrogen diffusion and embrittlement of multiphase fine-grained steel with increased plasticity and strength. Chem Biochem Eng Q 2011; 25:159-69.
[4] Hadžipašić AB, Malina J, Ni_znı´k S. The influence of microstructure on hydrogen diffusion in dual phase steel. Acta Metall Slovaca 2011; 17:129-37.
[5] Haq AJ, Muzaka K, Dunne DP, Calka A, Pereloma EV. Effect of microstructure and composition on hydrogen permeation in X70 pipeline steels. Int J Hydrogen Energy 2013; 38: 2544-56.

[6] Hung HM, Ai JH, Scully JR. Effects of prior cold work on hydrogen trapping and diffusion in API X-70 line pipe steel during electrochemical charging. Corrosion 2014; 70:166-84.

DSL310
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Effect of the Submicrocrystalline State Formation on the Diffusion of Hydrogen in Titanium

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Comparative studies of the hydrogen diffusion in coarse-grained (average grain size 80 mm) and submicrocrystalline (average size of grain-subgrain structure elements 0.12 mm) titanium were carried out by means of membrane method by combination of the electrolytic cell with high-vacuum chamber and mass spectrometer. Submicrocrystalline state in titanium was obtained by the method combined equal channel angular pressing (8 passes at temperatures of 673...573 K) and cold deformation by rolling to 75 % (change of blank thickness). Effective constants of hydrogen diffusion were determined from the intensity curves representing change of hydrogen content (penetrated through coarse-grained and submicrocrystalline titanium membranes during electrolysis) in the vacuum chamber.

Values of diffusion constant for submicrocrystaline titanium are lower (by 2–3 times) than corresponding values for coarse-grained titanium and decrease with increasing dislocation density in the bulk of submicrocrystalline structure. s mass of hydrogen in vacuum chamber reaches the steady-state level, the concentration of hydrogen in submicrocrystalline titanium membranes becomes 3 times higher compared to the coarse-grained state. It indicates the greater capability of submicrocrystalline titanium for hydrogen accumulation in bulk of the material in comparison with coarse-grained state. Decrease of effective constant of hydrogen diffusion and increase of capability of titanium submicrocrystalline structure to accumulate hydrogen in bulk of the material in comparison with coarse-grained structure are shown to be predominantly caused by larger extension of grain boundaries.

DSL315
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Effect of Thermo Hydrogen Treatment on Lattice Defects in Zr-1Nb Alloy

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The influence of hydrogen sorption-desorption cycles on defect structure of Zr-1Nb alloy was investigated. Specimens were hydroganated from gas atmosphere at temperature 500 °C and pressure 2 atm up to the hydrogen concentration equal to 0.05 wt.% for each cycle. The hydrogen concentration during saturation was determinate by the volumetric method. Then samples were annealed at temperature 900 °C with the heating rate of 4 °C/s. The lattice defects were studied by means of positron lifetime spectroscopy (PLS) and Doppler broadening spectroscopy (DBS). New experimental data about the evolution of the positron annihilation parameters τ_1, τ_2 and their corresponding intensities I_1, I_2, as well as the relative changes in the parameters S/S_0, W/W_0 depending treatment stage in Zr-1Nb alloy during thermo hydrogen proccessing was obtained.

DSL358
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Influence of the Confinement Dimension on the Diffusion of Molecular Hydrogen Confined into Ice Clathrates
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Safe and effective hydrogen storage is widely recognized as a key technology for hydrogen economy in the 21st century, with porous materials being one of the highly potential storage media. However, it proved to be challenging to achieve target goals in 2015 set up by DOE for hydrogen storage systems. Systematic studies of the storage processes are needed for fundamental understanding of storage mechanism as a basis for the successful synthesis and design of new materials. We have studied the effect of the confinement dimension on the diffusion of the molecular hydrogen in clathrates hydrates using neutron spectroscopy. Clathrates hydrates are nanostructured porous materials with nanocages of various sizes and with maximal H_2 storage capacity of 5.3 wt% [1]. They present particularly suitable model systems to study the impact of confinement since the interactions between ice-based clathrates framework and H_2 in cages are of the same hydrophobic nature. We observed strong differences of the diffusion and microscopic mobility of H_2 depending on the confinement size. In the "small" cage of 0.75 nm average diameter the motion of H_2 is strongly localized in the center of the cages even at temperatures up to 200K [2]. Moderate increase of the confinement dimension to 0.946 nm changes the behavior of H_2 dramatically and leads to the onset of the diffusive motion already at T=10K [3]. Such differences in microscopic dynamics help to explain the differences in the macroscopic parameters such as sorption pressure and hydrogen release temperature. Similar effect was also observed in the porous carbon [4]. The reduction of the pore size to 0.8 nm leads to strong decrease of the diffusion of confined hydrogen with obtained diffusion coefficient of about 2.35 ±0.7 Å2/ps at 100K. This is only the third of the diffusion coefficient measured at nanohorns at 25K with confinement dimension of 8 nm [5].

[1] W.L. Mao, H.K. Mao, A.F. Goncharov et al, Science 297, 2247 (2002) and J. S Tse, D.D. Klug, J.Y. Zhao et all, Press, W. Nat. Mater. 4, 917 (2005);
[2] E. Pefoute, E. Kemner, J. C. Soetens, A. Desmedt, M. Russina, J. of Phys. Chem. C, 116, 16823 (2012)
[3] M. Russina, E. Kemner, F. Mezei, in press
[4]. H. Kürig, M., Russina et al, in preparation
[5] F. Fernandez-Alonso et al, PRL 98, 215503 (2007)

VIP045
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The Role of Hydrogen Interaction with Defects like Vacancies, Dislocations and Grain Boundaries and its Relevance for Hydrogen Embrittlement
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Models on hydrogen embrittlement relying on hydrogen induced defect generation are reviewed. It will be shown that they are based on a recently developed novel thermodynamic analysis called defactant concept [1,2,3]. Like surfactants decrease surface energies defactants are solute atoms which decrease defect energies and, therefore, increase the rate of defect generation and mobility. In this concept the chemical potential of hydrogen is the most appropriate quantity as its increase leads to an increase of defect production. The novel concept allows to comprehend experimental results showing that (i) high vacancy concentrations can be reached in metals during severe plastic deformation and at high hydrogen fugacities [4, 5], (ii) dislocation nucleation is remarkably decreased in the presence of hydrogen [6,7] and (iii) high pressure torsion leads to nanocrystalline Pd-H alloys. In addition, dislocation mobility is enhanced by solutes leading to solid solution softening [7], if the solute segregate to dislocation kinks and if the mobility is determined by kink pair formation. Thus the defactant concept provides a thermodynamic rationale for the HELP (hydrogen enhanced local plasticity) and the AIDE (adsorption induced dislocation emission) models. It also forms the basis of models relating embrittlement to the creation of new surfaces (crack opening) or voids (in front of the crack-tip).

[1] R. Kirchheim, Acta Mater. 55 (2007) 5129 and 5139
[2] R. Kirchheim, Int. J. of Materials Research 100 (2009) 483-487
[3] R. Kirchheim, Scripta Mater. 62 (2010) 67
[4] Y. Fukai: Physica Scripta T 103 (2003) 11
[5] M. Krystian, D. Setman, B. Mingler, G. Krexner, M.J. Zehetbauer, Scripta Mater. 62 (2010) 49
[6] A. Barnoush and H. Vehoff, Acta Mater. 58 (2010) 5274
[7] E. Tal-Gutelmacher, R. Gemma, C.A. Volkert, R. Kirchheim, Scripta Mater. 63 (2010) 1032

VIP046

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Selective Hydrogenation of Multi-Unsaturated Hydrocarbons over Pd: New Mechanistic Insights
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Atomistic–level understanding of surface processes is a key prerequisite for rational design of new catalytic and functional materials. In our studies, we investigate mechanisms, kinetics and thermodynamics of heterogeneously catalyzed reactions and adsorption processes on nanostructured model supported catalysts to provide fundamental insights into the surface chemistry. By employing pulsed multi-molecular beam techniques, IRAS and synchrotron-based spectroscopies on Pd/Fe3O4/Pt(111) model surfaces, we study mechanistic details of complex multi-pathway surface reactions, such as hydrocarbon transformation in presence of hydrogen or selective hydrogenation of multi-unsaturated hydrocarbons.

Particularly, we investigate the interaction of α,β-unsaturated ketones isophorone and acrolein and their derivatives on supported Pd nanoparticles and extended Pd(111) surface. It could be shown that the selectivity in hydrogenation of C=O vs. C=C bonds in these compounds critically depends on the chemical composition of the adsorbate overlayers formed on Pd surfaces under the reaction conditions. Thus, selective hydrogenation of C=O bond in acrolein was observed over Pd(111) surface, while only C=C bond hydrogenation could be detected over Pd nanoparticles. These differences in the reactivity can be traces back to the different hydrocarbon spectator species formed in the induction period prior the onset of the product formation. Specifically on Pd(111), acrolein was found to form a dense hydrocarbon layer resulting from partial hydrogenation of the reactant. This layer formed in the induction period serves as a modifier, which renders the surface to be highly selective in C=O bond hydrogenation. On Pd nanoparticles, formation of such hydrocarbon layer is prevented by strong acrolein decomposition and the surface remains active only to hydrogenation of the C=C bond. The underlying mechanistic picture of these surface processes will be discussed.

DSL269
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Quantum Simulations for Hydrogen Isotope in Materials
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The first principles calculation based on the density functional theory is one of the most successful and powerful methods in the materials physics. And also the first principles molecular dynamics simulation methods have been used for various dynamical behaviors. The diffusion phenomena in solids and liquids are also the targets of such an ab initio simulations. In the case of small mass atoms like hydrogen atoms, we should treat their light nuclei in a quantum-mechanical manner, in addition to electrons. The quantum behaviors of the nuclei have crucial roles to play in the materials related to today's energy technology: fuel cell and lithium-ion rechargeable battery, not only from their academic interests [1-7]. Positive muon is also one of our target quantum particles, because it has been used as the probes to observe the states and motion of H and Li in materials, mu-SR[8-10]. The positive muon has the same spin and same charge as a proton and behaves as the lighter isotope of light hydrogen, which has ninth mass of proton. It is important to analyze the quantum behavior of these particles in the materials. We have been developing the quantum simulation codes, "Naniwa", for the small mass atom nuclei and positive muon on solid surfaces, in subsurfaces and bulk crystals [1-3] with the aid of the first principles calculations. In the conference, we will show our simulation results for hydrogen isotopes in materials, and discuss the quantum mechanical effects of these particles [3-7].

[1] H. Kasai, et al., Progress in Surface Science, 44 (1993) 101.
[2] W. A. Diño, et al., Progress in Surface Science 63 (2000) 63.
[3] K. Nobuhara, et al., Surface Science, 507-510, (2002) 82.
[4] T. Roman, et al., e-J. Surf. Sci. & Nano., 4 (2006) 619.
[5] N. Ozawa et al., Surface and Interface Analysis, 40 (2008) 1108.
[6] A. D. Pant et al., JPS Conf. Proc. 2 (2014) 010313.
[7] K. Shimizu et al., J. Phys. Soc. Jpn. 83 (2014) 013601.
[8] S. F. J. Cox, Rep. Prog. Phys. 72 (2009) 116501.
[9] K. Shimomura et al., Phys. Rev. Lett. 89 (2002) 255051.
[10] J. Sugiyama et al., Phys. Rev. Lett. 103 (2009) 147601.

DSL273
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Numerical Analysis of the Influence of Grain-Boundary Characters Distribution on Hydrogen Diffusion in Polycrystalline Materials
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The diffusion of hydrogen in metals is a key factor for understanding the basic mechanisms of hydrogen embrittlement. Numerous parameters affect this phenomenon, such as hydrogen trapping or the presence of a surface layer [1]. In addition, the character and distribution of grain boundaries is known to affect the macroscopic data determined experimentally, such as hydrogen diffusion coefficient [2]. Despite the large documentation about the subject, there are no studies showing a direct correlation between the grain-boundary characters distribution and the hydrogen macroscopic diffusivity, in particular because of the variety of interconnected grain boundaries. In this numerical work, we present an analysis of the effect of grain boundaries spatial distribution and connectivity on hydrogen macroscopic diffusivity, by considering grain boundaries either as diffusion short-circuits or preferential trapping sites. To understand these phenomena, permeation tests [3] were simulated using the finite element method (FEM), for regular hexagonal 2D-microstructures. The modelled membranes contain several phases (grains, random/sigma grain boundaries) with different diffusion properties.

Firstly, a statistical characterization of grain boundary networks topology and connectivity is presented. Then, a correlation between hydrogen macroscopic diffusivity and the grain boundary networks parameters is proposed [4].

[1] E. Legrand, J. Bouhattate, X. Feaugas, and H. Garmestani, Int. J. Hydrogen. Energ. 37, 13574 (2012).
[2] A. Oudriss, J. Creus, J. Bouhattate, E. Conforto, C. Berziou, C. Savall, and X. Feaugas, Acta Mater. 60, 6814 (2012).
[3] M. A. V. Devanathan and Z. Stachurski, Proc. R. Soc. London Ser. A 270, 90 (1962).
[4] B. Osman Hoch, A. Metsue, J. Bouhattate, and X. Feaugas, Comp. Mater. Sci. 97, 276 (2015).

DSL353
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Analysis of Pressure-Composition-Isotherms for the Design of Hydrogen Permeable Metal Membrane

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The diffusion of hydrogen atom in metal membrane is generally the rate-limiting process of the total reaction of hydrogen permeation through them. Applying the Sievelts' law into the Fick's diffusion equation, the hydrogen permeation coefficient, $\square\square$ $(=D \times K)$ is derived and used as a measure to show the hydrogen permeation ability of metals and alloys, where D is the diffusion coefficient and K is the hydrogen solubility constant. However, there are many exceptional cases that the hydrogen flux cannot be analyzed with $\square$. This is because the hydrogen diffusion is not always driven by the gradient on the hydrogen concentration. Strictly speaking, the driving force for hydrogen diffusion is the gradient of the hydrogen chemical potential.

In this presentation, the following new description of hydrogen permeation [1] will be explained which has been derived from the diffusion equation based on hydrogen chemical potential. Also, some examples of the analysis of hydrogen permeability based on the new description and its application will be presented for Nb-based, V-based and Pd-based alloy membranes.

$$J = \frac{RTB}{2L} \int_{c_2}^{c_1} c \frac{d \ln P}{dc} dc, \qquad (1)$$

where J is hydrogen flux, R is the gas constant, T is absolute temperature, B is mobility for hydrogen diffusion, L is membrane thickness, c_1 and c_2 are hydrogen concentration at the feed and permeation sides of the membrane,

c is hydrogen concentration, P is hydrogen pressure. It is important to note here that the term "$d \ln P / dc$" reflects

the gradient of the pressure-composition-isotherm (PCT curve), meaning that the hydrogen flux, *J*, is linked with the shape of the corresponding PCT curve of the material.

[1] A. Suzuki *et al.* Int J Hydrogen Energy, 39 (2014) pp.7919-7924.

DSL357
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Ion-Beam-Based Diffusion Measurements of Deuterium in Tungsten near Room Temperature
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Permeation measurements are a well-established method to study the diffusion of hydrogen in metals. However, for materials with a low hydrogen permeability such as tungsten, the well-established approaches face several challenges. High temperatures and very thin samples are needed. Furthermore, the brittleness of tungsten and the acting forces due to the pressure difference as well as leak-tight clamping in a vacuum setup prevent reliable gas permeation measurements.

To overcome these problems, we present a plasma-based approach for hydrogen permeation studies on tungsten near room temperature that circumvents the problems described above and relies on an ion-beam-based detection method [1]. Few micron thin tungsten samples with a hydride-forming getter layer on one side are exposed to a deuterium plasma on the other side. The plasma implantation causes a very high sub-surface concentration of deuterium in the tungsten, which leads to a deuterium flux through the tungsten into the getter layer. The amount of deuterium stored in the getter is the integral of the permeation flux over the exposure time. The samples are then analysed using the nuclear reaction D(3He,p)4He. A series of measurements with different loading times yields the integral of the permeating deuterium flux over time, which can be used to calculate the lag time and thus the diffusion coefficient.

Such hydrogen isotope permeation studies are crucial for safety considerations regarding a future nuclear fusion reactor, for which tungsten is a promising plasma-facing material.

[1] W. Möller, B.M. Scherzer and R. Behrisch, Nucl. Instrum. Methods, 168, 289 (1980).

DSL367
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Formation and Degassing of Deuterium-Filled Blisters on Polycrystalline Tungsten
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Tungsten is a promising candidate for armoring the plasma-facing wall in a future nuclear fusion reactor because of its high melting point, low sputtering yield and low solubility for hydrogen isotopes, which are used as the fusion fuel. A side effect of the extremely low solubility is that if tungsten is supersaturated with, e.g., deuterium by plasma exposure, the formation of gas-filled cavities with corresponding surface features – often generally referred to as blisters – is observed under many exposure conditions. There are numerous reports about the occurrence of

blisters (see, e.g., [1] and references therein), and understanding of blistering phenomena on tungsten has made significant progress in recent years. Yet, many details of their nucleation, growth phase and the concomitant effects on the material are still not fully clear. However, these are necessary to extrapolate to conditions in a nuclear fusion experiment such as ITER. A common feature about many types of deuterium-induced blisters in tungsten is that their cavities are located far beyond the implantation range of the energetic particles from the plasma (see, e.g., [1, 2]). This contribution focuses on roughly spherical blisters that are created at grain boundaries oriented parallel to the surface of rolled tungsten exposed to laboratory plasmas (e.g., [1]). Typical exposure conditions are a deuteron flux of 1020 D/m2s, fluences between 1024 and 1026 D/m2, ion energy of 38 eV/D and sample temperatures between 300 and 500 K. First, a brief overview of their evolution with fluence and exposure temperature is presented. Then, the selection of specific grain boundaries for blister nucleation, the creation of defects by the growth of the blister, and the gas release from blisters during storage at room temperature as well as at elevated temperatures are addressed. For this, state-of-the-art methods such as confocal laser 3D microscopy, cross-section electron microscopy and isotope exchange experiments were used.

[1] M. Balden et al., J. Nucl. Mater 414(1) (2011) 69–72
[2] S. Lindig et al., Phys. Scr. T145 (2011) 014039

DSL393
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Kinetics of Hydrogen Adsorption and Solubility of Hydrogen in Nanoporous Palladium Prepared by Dealloying

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Hydrogen concentration-potential isotherms of nanoporous palladium with typical ligament size of 15nm prepared by dealloying were measured by means of the method of electrochemical loading at room temperature. The results (Fig. 1) show that, compared to bulk palladium, the solubility of hydrogen in a phase of the nanoporous palladium is enhanced about sevenfold and the miscibility gap is significantly narrowed, meanwhile the solubility in b phase is reduced, which is similar to other
nanostructured palladium[1,2]. The above characteristics regarding the solubility of hydrogen in nanoporous palladium can be quantitatively explained by the theory of relative sites fraction, namely, assuming that hydrogen occupies the surface and subsurface sites, and the fraction of surface and subsurface sites for hydrogen adsorption in nanoporous palladium can be calculated. Despite the fact that hydrogen show large solubility in a phase of the nanoporous palladium, the diffusion kinetics of hydrogen in the nanoporous palladium is rather sluggish. Based on an equivalent model, the effective diffusion coefficient of hydrogen (D) in nanoporous palladium was measured by means of the method of electrochemical stripping. The results indicate and D in the nanoporous palladium is much smaller than that in the bulk palladium, which can be explained by the trapping effect caused by the surface and subsurface sites with lower energy on hydrogen [3,4]. For comparisons, the solubility of hydrogen and the effective diffusion coefficient of hydrogen in the annealed nanoporous palladium with a larger ligament size of 40nm were also measured and all the results meet current conclusions and explanations mentioned above. With the measured diffusion coefficient and the newly developed equivalent model, the absorption kinetics of hydrogen in nanoporous palladium can be well described, see Fig. 2.
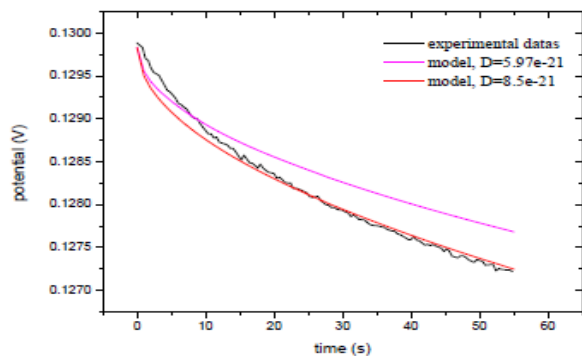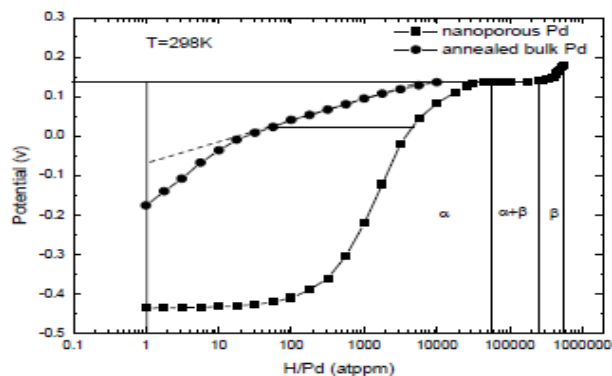
Figure 1 Concentration-potential isotherm of hydrogen in nanoporous palladium
Figure 2 Experimental and calculated potential drop due to hydrogen absorption

[1] T. Kuji, Y. Matsumura, H. Uchida, et al. Journal of Alloys and Compounds, 718 (2002).
[2] C. Sachs, A. Pundt, and R. Kirchheim, et al. Physical Review B, 64 (2001).
[3] T. Mütschele and R. Kirchheim, Scripta Metallurgica , 21 (1987).
[4] Y. Li and Y. T. Cheng, Int. J. Hydrogen Energy, 21 (1996).

VIP047
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Interactions of Hydrogen with Transition Metal Nanoparticles from First Principles

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Nanostructuring of transition metals can very strongly affect some of their properties related to interactions with hydrogen. Results of our density-functional modelling of bare and supported Pd, Pt, Ni and Rh nanoparticles containing different amounts of adsorbed and absorbed hydrogen atoms will be presented and compared with the results obtained for the corresponding extended (bulk) metal systems. In particular, we shall address: (i) binding of adsorbed and absorbed H atoms at various concentrations on bare and oxide-supported Pd and Pt nanoparticles [1,2]; (ii) effects on the surface chemistry of Pd by the interplay of C and H atoms [3,4]; (iii) how absorbed H can affect catalytic activity of transition metals [5].

[1] S.M. Kozlov, H.A. Aleksandrov and K.M. Neyman. Adsorbed and subsurface absorbed hydrogen atoms on bare and MgO(100)-supported Pd and Pt nanoparticles. J. Phys. Chem. C 118 (2014) 15242.
[2] S.M. Kozlov, H.A. Aleksandrov and K.M. Neyman. Energetic stability of absorbed H in Pd and Pt nanoparticles in a more realistic environment, submitted.
[3] K.M. Neyman and S. Schauermann. Hydrogen diffusion into Pd nanoparticles: Pivotal promotion by carbon. Angew. Chem. Int. Ed. 49 (2010) 4743.
[4] H.A. Aleksandrov, F. Viñes, W. Ludwig, S. Schauermann and K.M. Neyman. Tuning surface chemistry of Pd by atomic C and H: A microscopic picture. Chem. - Eur. J. 19 (2013) 1335.
[5] H.A. Aleksandrov, S.M. Kozlov, S. Schauermann, G.N. Vayssilov and K.M. Neyman. How absorbed hydrogen affects catalytic activity of transition metals. Angew. Chem. Int. Ed. 53 (2014) 13371.

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First-Principles Studies of Electrochemical Electrode/Electrolyte Interfaces

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In spite of its technological relevance in energy conversion and storage, our knowledge about the microscopic structure of electrochemical electrode-electrolyte interfaces is still rather limited. Due to the complexity of these interfaces a realistic description is theoretically and numerically rather challenging as proper thermal averages have to be performed and varying electrode potentials have to be taken into account [1]. These challenges will be briefly discussed but also promising routes to overcome them in the the framework of periodic quantum chemistry methods will be introduced.

I will in particular focus on the equilibrium coverage of metal electrodes with anions and cations in the presence of an aqueous electrolyte. The equilibrium ion coverage can be estimated by using a thermodynamic approach without taking the electrochemical environment explicitly into account. This approach will be illustrated using the adsorption of halide anions on metal electrodes [2]. At low electrode potentials, Pt(111) is usually hydrogen covered which influences the water structure which will be demonstrated using ab initio molecular dynamics studies [3]. Aspects of electrocatalytic reactions involving hydrogen such as the hydrogen evolution reaction will be discussed, The results for explicit water layers will be contrasted with calculations for an implicit solvent model [4] which is numerically very attractive as the water molecules are replaced by a polarizable dielectric medium but whose adequacy and reliability needs to be checked.

[1] N. Hörmann et al., J. Power Sources 275, 531 (2015).
[2] F. Gossenberger, T. Roman and A. Groß, Surf. Sci. 631, 17 (2015).
[3] T. Roman and A. Groß, Catal. Today 202, 183 (2013).

VIP053
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Interactions between Defects and Hydrogen Diffusion/Trapping Processes:
Some Impacts on Hydrogen Embrittlement in Polycrystalline and Martensitic Microstructures

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The impact of dislocation and vacancies distribution on hydrogen diffusion and trapping mechanisms have been investigated in a wide range of metallurgical states (grain-boundaries, dislocation patterns, martensitic steels, nickel base alloys, …) and different stress-strain states (tensile and cyclic loadings, internal stresses, …). Hydrogen states in the material depend mainly on the nature of the dislocation organizations and defects densities. The consequence of both on hydrogen embrittlement (HE) is illustrated and discussed in relation with diffusive and trapping hydrogen for two situations: inter-granular embrittlement of nickel base alloys and different crack modes observed on martensitic steels. Particularly, we illustrate first the effects of the Random and Special boundaries on the different defects and trapping sites stored in the grain-boundaries, and their consequences on hydrogen transport and segregation [1-3]. High-angle Random boundaries (R) are considered as a misorganized phase where the hydrogen diffusion is accelerated, while the Special boundaries (Coincident Site Lattice, CSL) constitute a potential zone for hydrogen trapping due to the high density of trapping sites as dislocations and vacancies. The predominance of one phenomenon depends on several parameters, such as the grain size, the probability of grain boundaries connectivity, the grain boundaries energy and the excess of free volume [1,2]. Additionally, our experiments confirm that hydrogen promotes vacancies formation probably in grain-boundaries. Tensile strengthening is reduced under hydrogen flux when the proportion of random grain boundaries increases [3]. This result supports the idea that hydrogen flux promotes intergranular fracture more than the hydrogen concentration. In a second part, we have questioned the hydrogen transport and trapping phenomena in different martensitic steels under an applied stress [5-10]. Both aspects can be affected by stress-strain states at different microstructural scales. Elastic distortion and plastic strain are both aspects of the mechanical states associated with defects (vacancies, dislocations), metallurgical elements (grain boundaries, precipitates), internal stresses and applied stresses, which can modify the diffusion and solubility of hydrogen. In the present work we first explore the effects of a tensile stress applied on martensitic steel membrane on the hydrogen concentration and mobility [7-8]. In a second part, we analyse the impact of mobile and trapped hydrogen on HE using local approach of fracture under hydrogen flux [9-10]. We clearly show that only mobile hydrogen can explain the quasi-cleavage observed for the martensitic steels.

[1] Oudriss, A., Creus, J., Bouhattate, J., Conforto, E., Berziou, C., Savall, C., Feaugas, X. (2012) Acta Mater., 60 (19), 6814-6828.

[2] Osman Hoch, B., Metsue, A., Bouhattate, J., Feaugas, X., (2015) Comp. Mater. Science, 97, 276-284.

[3] Metsue, A., Oudriss, A., Feaugas, X., (2014) Philosophical Magazine, 94 (34), 3978-3991.

[4] A. Oudriss, J. Bouhattate, C. Savall, J. Creus, X. Feaugas, F.A. Martin, P. Laghoutaris, J. Chêne (2014) Procedia Materials Science, 3, 2030-2034.

[5] Frappart, S., Feaugas, X., Creus, J., Thebault, F., Delattre, L., Marchebois, H., (2010) J. of Physics and Chemistry of Solids, 71 (10), 1467-1479.

[6] Frappart, S., Oudriss, A., Feaugas, X., Creus, J., Bouhattate, J., Thébault, F., Delattre, L., Marchebois, H. (2011) Scripta Mater., 65 (10), 859-862.

[7] Frappart, S., Feaugas, X., Creus, J., Thebault, F., Delattre, L., Marchebois, H., (2012) Mater. Sci. and Eng. A, 534, 384-393.

[8] Guedes, D., Oudriss, A., Frappart, S., Courlit, G., Cohendoz, S., Girault, P., Creus, J., Bouhattate, J., Metsue, A., Thebault, F., Delattre, L., Koschel, D., Feaugas, X., (2014) Scripta Mater., 84-85, 23-26.

[9] Oudriss, A., Fleurentin, A., Courlit, G., Conforto, E., Berziou, C., Rébéré, C., Cohendoz, S., Sobrino, J.M., Creus, J., Feaugas, X., (2014) Mater. Sci. and Eng. A, 598, 420-428.

[10] D. Guedes, A. Oudriss, S. Cohendoz, J. Creus, J. Bouhattate, X. Feaugas, F. Thebault, D. Koschel, (2014) Procedia Materials Science, 3, 2024-2029

Special Session 11
MICROSCOPY, MICROANALYSIS AND THEIR APPLICATION ON MATERIALS (SS11)

VIP065
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Evaluation of the Microstructure and Charpy Impact Toughness of Hot Worked Powder Ti-6Al-4V

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Ti-6Al-4V powder, produced by the hydride-dehydride (HDH) process, was hot isostatic pressed (HIP) into three bars. The 4in diameter bars were hot worked (HW) to three different diameters: 2in. (75% Rolling), 1.5in. (86% Rolling), and 1in. (94% Rolling). Three samples were machined out of each bar along the end, middle and transverse orientations. These samples were ground, polished, and etched. The microstructure of the samples was evaluated at 100X and 200X magnifications. The objective of this experiment was to examine the effect of deformation on the microstructure and properties of hot rolled titanium alloy bar product. The microstructure was characterized by the grain size and shape measurements as a function of the amount of deformation. The crystallographic texture was analyzed by producing (0002) pole figures. Charpy Impact samples were also machined out of each of the various diameter bars. Impact testing was used to quantify toughness by correlating the microstructure to the energy absorbed. Scanning electron microscopy (SEM) was performed on the fractured surface of the Charpy Impact samples.

Keywords: Ti-6Al-4V powder, HDH process, Hot Working, Charpy Impact toughness, Texture analysis.

DSL219
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Precipitation Processes in Hot-Rolled Al–Mn–Sc–Zr Alloy

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The effect of hot rolling on mechanical and electrical properties, microstructure and recrystallization behaviour of the AlMnScZr alloy was studied. The as-cast alloy and the alloy after hot rolling at 300 °C was studied during step-by-step quasilinear annealing from 200 °C up to 600 °C with heating rate 100 K/h followed by subsequent isothermal annealing at 600 °C/4 h. Precipitation reactions were studied by electrical resistometry and (micro)hardness measurements. Transmission, scanning electron microscopy and electron backscatter diffraction examinations of specimens quenched from temperatures of significant resistivity changes were used to identify microstructural processes responsible for these changes. Only occasional irregular sharp-edged polygonal particles of the AlMnFeSi system were found in the as-prepared state of the as-cast alloy. The as-prepared state of the hot-rolled alloy was characterized by a dispersion of fine coherent Al3Sc and/or Al3(Sc,Zr) particles, and

furthermore a fine (sub)grain structure was observed. The hardening effect in both alloy is due to presence and/or precipitation of the Sc,Zr-containing particles with L12 structure. The distinct resistivity changes of the alloys are mainly caused by precipitation of Mn-containing particles. The presence of Sc,Zr- and Mn-containing particles has an antirecrystallization effect that prevents recrystallization at temperatures minimally up to 600 °C/1 h. The phase development of the hot-rolled AlMnScZr alloy consists of the additional precipitation and/or coarsening of Sc,Zr-containing particles with L12 structure from the Al–Sc–Zr system. The process is accompanied and/or followed by the formation of Mn,Fe-containing particles. The apparent activation energy for the additional Al3(Sc,Zr)-phase and Al6Mn-phase precipitation in the hot-rolled alloy was also determined. The results obtained in the hot-rolled AlMnScZr alloy are comparable to those observed in the AlMnScZr alloy after extrusion at 350 °C studied in our previous work.

VIP032
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Characterization of Graphene Oxide Obtained from Alternatives Sources
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The unique atom-thick and two-dimensional structure of graphene has excellent mechanical and electronics characteristics [1]. Currently the best way to obtain graphene is the graphene oxide (GO). The first preparation of GO was done by the chemist Benjamin C. Brodie in 1859 by treating graphite with a mixture of potassium chlorate an fuming nitric acid [2]. Another method of obtaining GO has been the chemical exfoliation of graphite using the Hammers' method [3] or the improved method of Hammers [1]. Until 2004, Novoselov and Gueim [4] obtained a film of graphene mechanically exfoliating graphite and subsequent oxidation. The redox method of graphite has shown promise in producing films of GO on a large scale. However, is a very exothermic process that liberates gas harmful to the environment and humans persons. This article deals with the characterization of graphene oxide from alternative sources of carbon and dry method. Comparative studies with Raman spectroscopy suggest that this way is promising and more eco-friendly. We developed a fast and economic method to produce GO without toxic gasses like produced in Hammers method [1]. The results obtained in this study were equal or very close to those obtained in the indicated literature.

References
[1] J. Chen, B. Yao, C. Li and G. Shi, "An improved Hummers method for eco-friendly synthesis of graphene oxide," J.Carbon, vol. 64, pp. 225-229, 2013.
[2] B. Brodie, "On the Atomic Weight of Graphite," Philosofical Transations of the Royal Society of London, pp. 149-249, 1859.
[3] R. E. Offeman and W. S. H. Jr, "Preparation of graphitic oxide," Journal of the American Chemical Society, vol. 80, p. 1339, March 1958.
[4] K. S. Novoselov, A. K. Geim and S. V. M. e. al, "Electric field in atomically thin carbon films," Science, vol. 306, pp. 666-669, 2004.

DSL094
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Analysis of Microstructural Characteristics and Elemental Distribution across the Interfacial Zone of Diffusion Bonded γ-TiAl and Ti-22Al-25Nb Alloy

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In the present investigation microstructural aspects and elemental distribution characteristics of interface zone solid-state diffusion bonding of Ti-47Al-2Nb-2Cr (γ-TiAl) intermetallic with Ti-22Al-25Nb alloy has been carried out at high vacuum. Characteristics of the elemental distribution across the interface and constituent phases at the interfaces were analysed by using electron probe microanalysis (EPMA). Scanning electron microscopy (SEM) together with electron backscattered diffraction (EBSD) technique has been used to analyse the interfacial microstructure formed during the diffusion bonding. Effects of different diffusion annealing treatments on the evolution of microstructure at the bonding interface and element concentration at various distances from the bonding interface are also emphasized in the present study.

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DSL215
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Effect of Interfacial Heat Transfer Coefficient on Dendritic Growth and Microhardness During Horizontal Directional Solidification of an Aluminum-Copper Alloy

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The prediction of interfacial heat transfer coefficient (hi) is of great interest for the evaluation and design of the structure, properties and performance of solidified products so that the determination of this coefficient during directional solidification of metallic alloys can be considered as an important object of investigation [1-2].
This paper presents a theoretical-experimental study for the prediction of hi during the horizontal directional solidification of an Al-3wt.%Cu alloy on water cooled stainless steel chill under transient heat flow conditions. Eight thermocouples were connected with the casting and the time–temperature data were recorded automatically. The thermocouples were placed at 5, 10, 15, 20, 30, 50, 70 and 90 mm from the interface. A numerical technique [2] which compares theoretical and experimental thermal profiles was used to measure the hi values. This has permitted the evaluation of the variation of metal-mold heat transfer coefficient along the solidification which is represented by a power equation that shows the time dependence during the process given by hi = constant (t)-n, which represents the best fit between the experimental and calculated curves. The obtained results also include the variation of primary (λ_1) and secondary (λ_2) dendritic arm spacings of investigayed alloy as a function of hi. In

order to have the λ1 and λ2 measured, samples were extracted from the casting and analyzed by optical microscopy. The primary and secondary dendrite arm spacings were found to decrease as hi values are increased. Finally, an experimental law of Hall-Petch type is proposed relating the resulting microhardness (HV) to the hi.

[1] W.D. Griffiths, Metall. Mater. Trans. B, 31, 285 (2000).
[2] J.N. Silva, D.J. Moutinho, A.L. Moreira, I.L. Ferreira and O.L. Rocha, Mater. Chem. Phys., 130, 179 (2011).

DSL274
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Parallelization Solver for Kinetic Monte Carlo Precipitation Simulation of Bcc and Fcc Lattices

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Kinetic Monte Carlo (kMC) is an extremely powerful method to simulate the time evolution of Markovian processes. kMC relies on the a priori knowledge of a given set of transition rates characterizing the simulated processes. Because of its versatility, ease of implementation, and wide range of applications, kMC has been the object of a significant parallelization effort in order to take advantage of existing and upcoming peta- and hexa-scale computing capabilities. However, the difficulty of parallelizing kMC lies in the intrinsic time discreticity underlying event driven simulations, which are sequential in character, and do not lend themselves to trivial parallel implementations [1].

In this paper we describe the design of a synchronous parallel kinetic Monte Carlo (spkMC) algorithm in detail, giving some insight to specific simulation details such as the treatment of boundary conflicts, the replication of vacancies, and the communication model. We will validate the algorithm to determine its overall performance, precision, scalability (processor and memory usage), and inter-process communication performance, by solving well-understood diffusion problems: nucleation of precipitates.

The spkMC strategy is based on: 3D lattices (BBC: body-centered cubic or FCC: face-centered cubic systems) decomposed in 3D grids of subdomains, each subdomain is further divided in 2×2×2 sectors, with these 8 sectors it will be implemented a checkerboard scheme that avoids boundary conflicts and simplifies kMC parallelization, a periodic synchronization among processes through a frequency line for each process events, at the synchronization points (end of a sprint) the changes that occurred in the boundary and ghost regions are communicated to the neighbour processes.

The simulation results include comparisons between kMC and spkMC algorithms, in terms of performance, precision and precipitates measures. The sequential and parallel simulations were run on the SeARCH cluster, located at the University of Minho.

The outcome of this work is a set of software applications written in C, that allows, (i) Monte Carlo (MC) simulations with and without MPI, (ii) result analyze using the Density Based Spatial Clustering of Applications with Noise (DBSCAN) technique [2], and (iii) compare the simulation results with the classical nucleation theory. Practical results obtained with these applications are (i) reports about the simulation, the analysis of clusters and precipitates; (ii) files for 3D visualization of the simulation, at various stages over time, before and after applying DBSCAN to clean unclustered atoms.

[1] E. Martínez, P.R. Monasterio, J. Marian, "Billion-atom synchronous parallel kinetic Monte Carlo simulations of critical 3D Ising systems," Journal of Computational Physics, pp. 520-531, 2011.
[2] M. Ester, H.-P. Kriegel, J. Sanders, and X. Xu, "Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise", KDD, 1996.

DSL338
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Contribution to the Study of the Electrochemical Behavior in Conducting Medium (Soil) of a Metallic Composite Material WC-W-Ni / Cu-Mn

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The PDC diamond tools (Polycrystalline Diamond Compact) used in oil drilling field contain two parts:
- The body of the matrix tool obtained by infiltration.
- The PDC wafer brazed to the tool's body. [1] [2]

This work focuses on the elaboration of new grades of the drill tool and study the matrix of electrochemically recent study under basic and acidic conditions, several techniques were used, including the polarization curves, resistance polarization, electrochemical impedance spectroscopy (EIS), we also studied the microstructural evolution of the mixture of WC / W / Ni powders in the infiltration of a metal binder, the cupermanganèse Cu-30Mn-1P. The morphology and distribution of the elements constituting the matrix are established by SEM (Scanning Electron Microscope) coupled to the EDS (Energy Dispersive Spectroscopy). Concentration profiles and maps X established by EDS (Energy Dispersive Spectroscopy) are make in the direction of infiltration, phase identification was make by X-ray diffraction (XRD).

The electrochemical results shown that we have two capacitive loops in acid medium and a capacitive loop in basic medium with a decrease of the bias resistor to the shades less rich in WC, thus favoring the presence of similar corrosion process at the surface of each electrode.

[1] Jean-Paul Nguyen, Le Forage, Edition Technip Paris, p 53, (1993).
[2] F. Grondin, Les Outils de Forage, SONATRACH, p 6-7, 16-18, (2004).

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Experimental Study and Modeling of Low Temperature Tempering Processes

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Tempering is one of the diffusive phase transformations in steel alloys, it is used as an effective means to improve the ductility and toughness of hardened steels, and release residual stresses generated in components after hardening. In this paper, the effect of low temperature tempering on microstructures and mechanical properties of G50 steel which is a kind of cobalt free High Strength Low Alloy steels was investigated by using SEM, TEM and dilatometric tests. Using measured dilatation curves of low temperature tempering and changes of hardness before and after that process, a kinetic model of low temperature tempering processes in G50 steel was establish by introduction of a tempering parameter and an adopting JMA-type equation. The proposed model was used to predict low temperature tempering processes in G50 steel.

Keywords: Low temperature tempering, Diffusion, HSLA, Numerical simulation

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DSL379
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Microstructural and Mechanical Properties of Aluminium Matrix Tial Reinforced Composite Coatings Produced by Cold Spraying Process

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Scope of this study is investigation of the effect of titanium aluminide reinforcing particles to the mechanical and microstructural properties of aluminium based coatings produced by cold gas dynamic spraying process. For this purpose, titanium aluminide powder was produced by powder metallurgy route. Required amount of titanium and aluminium powder were compacted by uniaxial press and held at 750oC during 24 hour. Furthermore, aluminium powder is mixed with different ratios (0, 15, 30 vol. %) of titanium aluminide particles and sprayed on substrate surface. Microstructural characterizations of the coatings are performed with optical and scanning electron microscopes. X-Ray Diffraction analysis was executed to specify the different phases in the coatings. Hardness measurements and wear tests were conducted as mechanical tests to compare the performances of the coatings.

DSL390
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Nano Scale Study and Application of Microscopes in Enhance Oil Recovery: A Review

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Enhance oil Recovery (EOR) issues such as wettability alteration, particles transmission and retention, Interfacial Tension (IFT) reduction and fine migration have been of major concern to researchers and experts in recent years. Large number of unanswered question in this area still remain. Control, or improvement among these above mentioned parameters are not possible without fully understanding knowledge of mechanisms behind these process. For example wettability alteration is well known as main and key parameter for oil recovery factor (RF) increment in carbonate reservoirs. However wettability alteration mechanisms are not clear and a desirable altering in wettability alteration is infeasible.
This research is a review of the application of microscopes such as Transmission Electron Microscope (TEM), Scanning Electron Microscopic (SEM), Environmental scanning electron Microscope (ESEM), Fluorescence Confocal Microscope (FCM) and Atomic Force Microscopy (AFM) for more interpretation and analysis of governing

mechanisms in aforementioned EOR matters. This Study explore the use of these microscopes, Fourier Transform Infrared Spectroscopy (FTIR), Zeta potential and Flame atomic absorption spectroscopy (FAAS) together with surface chemistry knowledge of these EOR parameters to enable the breakthrough toward finding solutions for abovementioned problems.

[1] A. M. Munshi, V. N. Singh, Mukesh Kumar, and J. P. Singh J.Appl. Phys 103, 084315 (2008).
[2] P. McElfresh, D. Holcomb and D. Ector, SPE 154827, 12–14 June (2012).

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Atom Probe Tomography (APT) Combined with in-Situ TEM:
Impacts on the Electronic Memory Device Technology

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Solid-state microelectronics has been progressed for more than 50 years. As the size of device is getting smaller, the demands for both structural and compositional information in sub-nanometer scale are getting increased. Conventional analytical techniques, such as TEM and SIMS, for the structural and compositional analyses, however, revealed limitation in acquiring the three-dimensional information in sub-nanometer scale. Atom Probe Tomography (APT) technology has been developed to overcome the current technical limit of conventional analysis, and thus, to provide three dimensional distributions of constituent elements at sub-nanometer region with high detection sensitivity (~ppm).

Since the distribution of ppm-level constituent elements can play a critical role in the performance of recent electronic devices, 3D compositional information combined with structural information is quite demanding for understanding the device characteristics. This presentation will show various examples and discuss the impacts of APT analysis combined with in-situ TEM on the current researches of micro-electronic memory devices, such as DRAM (with STI and finFET structures), Flash Memory, PRAM (Phase Change Random Access Memory) and ReRAM (Resistive Random Access Memory).

VIP060
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Synthesis and Structural Properties of (Bi,Na)TiO3-(Bi,K)TiO3-BaTiO3 Lead-Free Piezoceramics

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In this work we report the processing and the structural characterization of the xBi0,5Na0,5TiO3 – (0,7186 – 0,7143x)Bi0,5K0,5TiO3 – (0,2814 – 0,2857x)BaTiO3 (BNBK1000x) lead-free piezoelectric ceramics with compositions x = 0.93, 0.912, 0.879, and 0.82 near to the morphotropic phase boundary (MPB). The BNBK1000x piezoceramics were obtained by conventional solid-state reaction, starting of analytical purity oxides and carbonates Bi2O3, Na2CO3, K2CO3, BaCO3 and TiO2. The powders were mixed, calcined in 850°C for 3 h, and then cold-pressed and conventionally sintered. The relative densities of the obtained ceramic samples were larger than 95%. Structural properties of BNBK1000x ceramics were investigated by scanning electron microscopy (SEM), X-ray diffraction (XRD) and Raman spectroscopy.

The SEM's result suggesting that all compositions are homogeneous and the grain size is dependent on the ions K+ and Ba2+ content. The X-ray diffraction patterns revealed that BNBK1000x ceramics presenta complex perovskite crystalline structure for all compositions studied, without traces of spurious phases or TiO2-nonstoichoimetry-induced secondary phase [1]. The comparison between XRD and Raman shift data showed that the effects of the ions K+ and Ba2+ incorporation in crystalline structure of the BNBK1000x were the increasing of the chemical disorder, common in Bi-based systems, and the possible mixture of rhombohedral (R3c) and tetragonal (P4mm) phases for composition in MPB [2].

[1] M. Naderer, T. Kainz, D. Schütz, K. Reichmann,J. Eur. Ceram. Soc., 34, 663 (2014).
[2] E-M.Anton,L. A. Schmitt, M.Hinterstein, J.Trodahl, B. Kowalski, W. Jo, H.-J.Kleebe, J.Rödel, J. L. Jones, J.Mater. Res., 27, 2466 (2012).

DSL255
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X-Ray Diffraction, Microstructure and Mössbauer Studies of Nanostructured Fe90Mg10 Powders Elaborated by Mechanical Alloying

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The mechanical alloying (MA) of elemental powder mixtures of Fe90Mg10 (atomic ratio of 79.67:20.33) was performed in an argon atmosphere using a planetary ball mill process. The alloy formation and different physical properties were investigated as a function of milling time, t (in the 0–54h range) by means of the X-ray diffraction (XRD) technique, scanning electron microscopy (SEM), and Mössbauer spectroscopy (MS). The formation of the solid solution α-Fe (Mg) started after 4 h of milling. The Mg peaks is completely missing. XRD results also indicated that when the milling time increases, the lattice parameter increases, whereas the grain size decreases and the mean level of microstrains increase. The powder particle morphology was observed by SEM at different stages of milling. The Mössbauer spectra were fitted with two sextets corresponding to the crystalline bcc Fe phase and a second sextet which represents supersaturated solid solutions of Mg in (α-Fe). The appearance and the increase in intensity of the second sextet 17, 66 % at (12 h) to 50 % (54 h) with t corresponding to the dissolved Mg in the (α-Fe). This may indicate that the interfacial region effect increases with milling time due to the grain size reduction and to the disordered state of the interfacial region.

[1] H. Reuther, M. Betzl, W. Matz and E. Richter, "Alloying by high dose ion implantation of iron into magnesium and aluminium" Hyp. Interact. 113 (1998) 391-401.
[2] H. Friedrich, S. Schumann: "Research for a new age of magnesium in the automotive industry", Journal of Materials Processing Technology, vol. 117 (2001) p. 276-281.

[3] G.S. Cole, A.M. Scherman: "Lightweight materials for automotive applications", Materials Characterization. vol. 35 (1995) p. 3-9.

[4] R. Fan, J. Sun, H. Gong, K. Sun, W. Wang: "Structural evolution of mechanically alloyed nanocrystalline Fe-28Al powders", Powder Technology, vol. 149 (2005) p. 121-126.

[5] Suryanarayana, C., Mechanical Alloying and Milling, Pro MaterSci., 2001, vol. 46, pp. 1–184;

[6] S. Mi and T.H. Countney, Processing Structure and Properties of Ni-W Alloys Fabricated by Mechanical Alloying and Hot – Isostatic Pressing.Scripta Mater, 1998, 38, p 637-677

[7] C.C. Koch and J.D.Whittenberger, Mechanical Milling/Alloying of IntermetallicsIntermetallics, 1996. 4. P 339-355

[8] A. Hightower, B. Fultz, R. C. Bowman, Jr.: Mechanical alloying of Fe and Mg, Journal of Alloys and Compounds 252 (1997) p. 238–244.

[9] E.P. Yelsukov, G.A. Dorofeev, A.L. Ulyanov: Mechanism and kinetics of mechanical alloying in an immiscible Fe--Mg system, Czechoslovak Journal of Physics, Vol. 55 (2005), No.7

[10] G.A. Dorofeev, E.P. Yelsukov, and A.L. Ul'yanov: Mechanical Alloying of Immiscible Elements in the Fe–Mg System. Inorg. Mater. 40 (2004) 690.

[11] Y. Yoneda, H. Abe, T. Ohshima and H. Uchida3: Phase transformation of Mg-Fe alloys. Journal of Applied Physics Volume 107, Issue 9, 1 May 2010, Article number 093505.

[12] High Score Plus Software, PAN alytical (2004).

[13] S. Vives, E. Gaffet, C. Meunier, Mater. Sci. Eng. A366 (2004) 229–238.

[14] I. Lucks, P. Lamparter, and E.J. Mittemeijer, An Evaluation of Methods of Diffraction-Line Broadening Analysis Applied to Ball-Milled Molybdenum, J. Appl. Crystallogr., 2004, 37, p 300–311

[15] A. Patterson, the Scherrer Formula for X-Ray Particle Size Determination, Phys. Rev., 1939, 56(10), p 978–982.

[16] A.R. Stokes and A.C.J. Wilson, Diffraction of X-rays by Distorted Crystal Aggregates. I, Proc. Phys. Soc. Lond., 1944, 56, p 174.

[17] K. Lagarek, D. Rancourt, Recoil Software, Physics Department, University of Ottawa, Ottawa 1998.

[18] L. Castex, J.L. Lebrun, G. Maeder and J.M. Sprauel: Détermination de Contraintes Résiduelles par Diffraction des Rayons X, vol.22, Publications scientifiques et techniques de l'ENSAM, Paris, 1981, pp. 51–60.

DSL348
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A Buried Structure for Fabrication of Micro Materials by Electromigration

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Electromigration (EM) is the physical phenomenon of atomic diffusion by electron wind force. EM is known as the negative phenomenon for electronic devices because the formation of hillocks and voids induced by EM deteriorates a metal line, and many researches have reported various ways for preventing EM [1]. On the other hand, our research group has developed the fabrication technique for micro/nano materials by utilizing EM [2]. The EM technique for fabricating micro materials has unique characteristics. The properties of materials fabricated by EM technique are in single crystal, pure material and high-aspect ratio. Additionally, the cross-sectional shape of micro material can be controlled by changing the shape of a hole for discharging atoms. Recently, the conductive passivation made of TiN was introduced for enhancing the fabrication of Al micro materials [3]. The passivation is one of the most important components within sample structure for fabricating materials. The multiple micro materials were fabricated by using conductive passivation. However, since the conductive passivation is deposited onto the whole surface of a Si wafer having the objective Al lines, current leaks out of the Al lines. Countervailing measure for precluding the leak of current is required. In this work, we develop a new structure, which is constituted of Al line buried in Si wafer, for preventing the leak of current and for advancing the fabrication technique utilizing

EM. The accumulation of metallic atoms caused by EM is shown and fabrication of micro material is demonstrated by the new structure. We report an advantage of the new structure in comparison with the previous one.

[1] K.N. Tu, J. Appl. Phys., 94, 5451 (2003).
[2] M. Saka and R. Nakanishi, Mater. Lett., 60, 2129 (2006).
[3] Y. Kimura and M. Saka, Mater. Lett., 116, 278 (2014).

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Fabrication of Microlens Array Obtained by Anisotropic Wet Etching of Silicon

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This paper present the fabrication of a microlens array surface with a single-mask process and two etching step with KOH water solution. Numerical analysis of optics was used to determine the optimal design parameters such as sagitta and radius of curvature. The dimension of each lens is 20µm x 20µm. We used anisotropic etching of <100> silicon through a circular and squar mask to produce a pyramidal pit formed by four (111) plane. The oxide mask is stripped and immersion of the sample in the etchant solution favors the etching of (411) plane that transforms the pit into a smooth hemispherical cavity. An intermediate stage exists when a wider 19.470 <411> -face pyramid replaces the initial 54.740 inverted pyramid. The dependence of surface roughness on concentration and temperature of KOH is investigated in range of 25%-40% and 600C-800C, respectively, and compared between them. The surface profiles and roughness was characterized by AFM. The etching depth and radius of micro-lens array was obtained from the SEM images and AFM data. Also, the array of cancave depressions was directly used as a mould for replication of transparent polymeric silicon KER 2500 from Shinetsu with refractive index n=1.41. The perfectly matched array of microlenses can be detached from substrate and used as a local solar concentrator. Optical properties such as the focal length of plano-convex microlens array which are obtained by replication, are measured and analyzed.

DSL377
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Fabrication of Foam Type Porous Silicon Carbide without Crack and Hollow Strut

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Foam type porous silicon carbide (SiC) ceramics without crack and hollow strut were fabricated by polymer replica method using polycarbosilane (PCS) and polyurethane foam as the starting materials. The synthesized porous SiC were analyzed by X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and BET Analysis. The results revealed that porous SiC ceramic formed with dense framework at a low temperature of 1200℃. During the heat treatment process, PCS experienced an organic-inorganic transformation and finally converted to SiC ceramics. It was known that an organic-inorganic transformation of PCS was affected by curing condition which was the stage of silicon oxycarbide (SiOC) formation. In this study, he optimum curing condition was air atmosphere for 7h at 200℃.

[1] Y.J. Lee, S.R. Kim, Y. Kim, D.G. Shin, J.Y. Won and W.T. Kwon, J. Kor. Ceram. Soc., Vol.51 (2014), p.1
[2] P. Colombo, G, Mera, R. Riedel and G.D. Sorarù, J. Am. Ceram. Soc., Vol.93 (2010), p.1805
[3] J.H. Eom, Y.W. Kim and I.H. Song, J. Kor. Ceram. Soc., Vol.49(2012), p.625
[4] M.R. Nangrejo and M.J. Edirisinghe, J. Porous Mater., Vol.9 (2002), p.131

DSL388
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Concurring Kinetics of Phase Transition and Grain Growth in Nanostructured Alloy

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Experimental observation and theoretical interpretation on the concurring kinetics of grain growth and phase transition in nanostructured Fe91Ni8Zr1 alloy were first presented. From in situ high temperature X-ray diffraction and differential scanning calorimetry, it can be confirmed that concomitant grain growth occurs and comes to a halt before phase transition is fully completed. From the currently kinetic description, grain growth not only adjusts the constitution of enthalpy change, but also influences the kinetics of phase transition. The present findings, offer a new behavior of phase transition owing to the size effect, and further, extend the understanding of the role grain boundary played in solid-state phase transition.

VIP018
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Microstructural Evolution and Thermal Stability of a Nanostructured SS304 Steel Fabricated by Ultrasonic Shot Peening

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Strain induced formation of nanostructured on the surface of metals were extensively reported in the last then years. Shot peening is one of the effective ways for fabricating nanostructures with severe plastic and compressive deformations, which retards crack nucleation/propagation. In the previous study of this group, the ultrasonic shot peening (USP) was applied on various pure metals, i.e., Fe, Ni, Cu, Al and stainless steels, aiming at the determination of the microstructural evolution mechanism. In addition to the surface nanocrystallization, another hot issue is the thermal stability of the surface nanostructured materials, since large portion of the treated materials are applied to elevated temperature range.

In this work, an engineering SS304 was subjected to USP, after peening, a gradient microstructure were fabricated on the surface, including the nanostructure, ultra-fine grain structure and coarse grain layer with the increase of depth from the treated surface. Specimens at different layer were heat treated at accelerated temperature of 500~700°C up to 6hrs, with subsequent microstructural investigation using transmission electron microscopy and so on. The fabricated nanostructure in the top layer showed a high stability even at 500°C. Detailed microstructural evolution will be presented in the talk.

[1] W.B. Liu C. Zhang, Z.X. Xia, J.M. Chen, Mater. Sci. Eng. - A 568, 176 (2013).

VIP065
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The Effect of Processing Method on Microstructure and Mechanical Behavior of Ti-6Al-4V Plate Produced by Powder Metallurgy Technique

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Three Ti-6Al-4V plate materials produced by powder metallurgy technique, included pre-alloyed hydride-dehydride (HDH) plate rolled to 75% reduction, and two blended elemental (BE) powder plates rolled to 75% and 87% reduction were evaluated. The objective of this study was to determine differences in microstructure and toughness between the pre-alloyed HDH and BE Ti-6Al-4V materials processed to the same product form. Heat treatments were performed below the beta transus temperature at 982, 871, 760, and 732°C (1800, 1600, 1400, and 1350°F) for 1, 2, and 4 hours in order to determine differences in heat treating response, and above the beta transus at 1076°C (1970°F) to determine the transformation temperature.

The samples were evaluated by scanning electron microscopy and optical microscopy. Charpy impact testing was performed in order to determine differences in the energy absorbed during fracture. (0002) pole figures of selected conditions were also performed in order to determine any differences in texture between the various conditions.

Special Session 12
NANOTECHNOLOGY IN OIL AND GAS (SS12)

DSL095
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The Study of Adsorption and Desorption Cycles with Heavy Diesel Sample using Ethanol as Solvent Leaching

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In recent years, there has been an increasing in the use of petroleum heavy fractions to produce fuels, such as diesel, due to the shortage of light crude oil for the production of these fuels. In Brazil, this problem is more serious, because besides Brazilian oil is a heavy oil, it contains a high nitrogen content (0.45 %) and low sulfur one (0.75 %) compared to international oils. Nitrogen compounds affect the catalytic activity of hydrotreating process (HDT), they contaminate the catalysts and decrease their lifetime and demand severe conditions for HDT. Therefore, it is required higher temperatures and hydrogen partial pressures, besides of a higher volume of catalytic reactor, which increases the cost of the process. Due to these factors, studies are being conducted aiming the removal of nitrogen compounds before HDT and adsorption is one of the processes that have been studied. However, the use of adsorption as an industrial process, it is necessary that the adsorbent to be regenerable. Thus, the aim of this work was to study cycles of adsorption and desorption, using a sample of heavy diesel and a commercial silica as adsorbent. The adsorption tests were conducted in a fixed bed, using a column of 24 cm height and 2.54 cm in diameter. The adsorption tests were performed at 80 °C and the desorption ones at 60 °C. It was used ethanol as solvent. It has been carried out fourteen adsorption and thirteen desorption tests. The results of the recovery test presented a reduction of approximately 20 % in the adsorption capacity of the adsorbent treated after the adsorption cycle compared to the fresh one. This result indicated that the silica sample can be reused.

Keywords: nitrogen compounds; adsorption; desorption.

DSL380
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Effect of Zinc Oxide Nanoparticle (ZnO NPs) Sizes on Viscosity in Enhanced Oil Recovery (EOR)

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The effect of ZnO NPs on the viscosity of nanofluid in potential EOR application was investigated. First the nanosized ZnO was synthesized using sol-gel method. The nanomaterials with structure were annealed at different temperatures ranging from 500 to 700°C which were chosen based on the Thermogravimetric (TGA) Analysis. The structure and morphology were characterized by Powder X-Ray Diffraction (PXRD) and Transmission Electron Microscope (TEM), respectively. The PXRD shows the increasing tendency in crystallite size when the annealing temperature increases and the hexagonal structure of ZnO. TEM further revealed the same tendency which the Zn NPs size increased with the annealing temperature. The ZnO nanofluid was then prepared with different particles sizes with the same concentration. Results revealed that the viscosity of the nanofluid increased 50% when the particles size increases from 40 to 80 nm with conserved density. The interfacial tension (IFT) also increased when the particle size increases. With the smaller size of NPs, we can obtain lower viscosity and which will help in increasing sweep efficiency to increase hydrocarbon production. Based on these analyses, it supports the theory claiming that nanoparticle can contribute for betterment in Oil and Gas industry especially in EOR [1].

[1] N.A. Ogolo, O.A. Olafuyi, and M.O. Onyekonwu, 8-11 April 2012, "Enhanced Oil Recovery Using Nanoparticles," Paper SPE 160847, presented at the SPE Saudi Arabian Section Technical Symposium and Exhibition.

DSL387
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Role of Brine Ions in Wettability Alteration during Surfactant Flooding In Oil-Wet Rocks

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Wettability alteration is well known as the main mechanism of producing oil in oil wet rocks. Indeed, spontaneous imbibition of the injected fluid in oil-wet reservoirs is slow because the grain surface has higher oil wettability than water, which causes early breakthrough to happen. Hence, Water flooding as a secondary recovery method in such cases is unsuccessful. Surfactant usage in injection phase is a well-known method for improving the wettability characteristics of the rock from oil-wet to a more desirable condition, water wet.

It is obvious that one cannot ignore the impact of brine salinity and ions on wettability alteration during surfactant flooding. However, not many researches have been conducted in that particular direction. Moreover, it is impossible to have a desirable wettability alteration without understanding the mechanisms behind the process.

This experimental investigation focused on the role of brine in wettability alteration and its mechanisms during surfactant flooding. The results show that the SO_4^{-2} plays an important role in decreasing the contact angle, at presence of cationic surfactant (1wt %), in such a way that increasing SO_4^{-2} concentration from 500 (ppm) to 6000 (ppm) in aqueous phase decreases the contact angle (wettability index) from 58° to 26°. Further results indicate that SO_4^{-2} is more effective in the presence of Ca^{+2} and Mg^{+2} ions.

[1] Morrow, N.R., G. Tang, M. Valat, and X. Xie, J. Pet. Sci. Eng., vol. 20, June, pp. 267-276 (1998).
[2] Aladasani, A. and Bai, B., SPE 152997, (2012).

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Improvement of an Iranian Oil Recovery in the GAGD Process using NanoSilica Particles

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Gas assisted gravity drainage (GAGD) is a novel subdivision of gas injection method. In this process the vertical injection wells are located in the upper bed of the oil zone, while the horizontal production wells are drilled at the bottom bed of the oil zone. This procedure is designed to take advantage of gravity between the injected gas and reservoir crude oil due to the difference in their densities.

Nanosilica particles were introduced as mobile adsorbents in oil reservoirs to adsorb the asphaltenes, reduce the viscosity and enhance the dispersion. The objective of this research is the experimental investigation of enhanced oil recovery using in situ nanoparticles for the first time using reservoir fluids. Moreover, nano-assisted and conventional GAGD processes were investigated to compare the asphaltene material deposition and ultimate oil recovery.

A 2-D Hele-Shaw physical model with $15 \times 67 \times 3$ cm dimensions was packed with uniform sandpacks to conduct visual experiments of GAGD Process. Sand grains were used in order to simulate the physical model as a sandstone reservoir rock with regard to the most of reservoir rocks in the world are in this type of geology. The permeability and porosity of visual model were 22 Darcy and 37%, separately. Dimensionless numbers such as Bond and Capillary number were applied to scaling conducted experiments to field range that were under gravity drainage mechanism of production.

Experiments were carried out using an Iranian offshore oil reservoir sample and carbon dioxide gas: the setup consisted of two sand-packed cells; one packed only with sand-packs as the oil matrix and the other with sand-packs and nanosilica, while they had similar porosity and permeability. The content of deposited asphaltene in swept matrixes, the interference between oil and gas, and oil recovery during GAGD process were monitored.

The results illustrated that nano-silica particles changed the matrix heterogeneity and led to improvement of asphaltene deposition distribution in the physical model that amount of asphaltene deposition was increased near injection well place but it was reduced near horizontal production well (more than 5.5%) so cause improve ultimate oil recovery (more than 7%).

Keywords: Nanosilica, Asphaltene Deposition, Gas Injection, Gravity Drainage, EOR, GAGD

DSL404
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A New Method to Estimate Model's Parameters for Foam Assisted Process using Genetic Algorithm
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Nowadays, foam assisted processes become one of the favorable subsets of enhanced oil recovery (EOR) mechanisms due to its low mobility comparatively to gas injection. In fact foam flooding improves gas flooding process due to reduction of gas mobility, consequently increasing sweep efficiency. In order to achieve a successful foam process, an appropriate model is required to predict the behavior of foam through porous media, correctly. There are several approaches for foam flow modeling through porous media [1]. Mechanistic approach is one of the most accurate as well as complicated among all approaches. However, some assumptions such as local steady state is applied to simplify the mechanistic model and this simplified model is usually used in simulation software.

In order to utilize local steady state model in simulation, various parameters are required to be determined by experiments. Different methods have been introduced in literature to derive foam model's parameters from steady state experimental data [2, 3]. Finding new method which is easier as well as faster than existing methods is the aim of this study.

In this study Genetic Algorithm is employed to derive model's parameters from a steady state data set. Although there are numerous parameters to be driven for simulation, but the simplest model is used in this study. These results are compared with the results of previous methods. The results demonstrate that implementation of Genetic Algorithm to determine foam model's parameters leads to reasonable values which can be applied in simulation of foam flooding.

[1] Hematpur H., Karimi M., Rashidi M., "A brief review on foam flow modeling through porous media", International Journal of Petroleum and Geoscience Engineering (IJPGE), 104-119, 2014

[2] Ma Kun, Lopez-Salinas J.L., Puerto M.C., Miller C.A., Biswal S.L., Hirasaki G.J., "Estimation of Parameters for the Simulation of Foam Flow through Porous Media, Part1: Dry-Out Effect", Energy Fuels Journal, May 2013.
[3] Rossen W.R., Boeiji, C.S. "Fitting Foam Simulation Model Parameters for SAG Foam Applications", SPE Enhanced Oil Recovery conference, Kuala Lumpur, Malaysia, July 2013.

VIP019
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Synthesis and Characterization of Yttrium Iron Garnet (YIG) Nanoparticles activated by Electromagnetic wave in Enhanced Oil Recovery

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Due to the geographical location and technological limitation, various novel enhanced oil recovery (EOR) methods has been proposed to recover the remaining oil from a depleted oil reservoir. Research on application of nanoparticles either by its own or coupled with other stimulating agent has been growing enormously and some of them has shown a promising future. Tackling problem arises in high temperature high pressure reservoirs have been chalenging with the existing chemical agents as thermal degradation will cause failure to the chemicals. In this work, temperature-stable YIG magnetic nanoparticles with electromagnetic wave has been proposed as a new candidate for reservoir stimulating agent. The purpose of nanoparticles injection is to increase the sweep efficiency in the reservoir by increasing the viscosity of displacing fluid. In this research, Yttrium iron garnet (YIG) nanoparticles has been injected into waterflooded oil saturated porous medium to recover the remaining oil in the presence of electromagnetic wave. At sintering temperature 1200°C, a mixture of hematite and YIG was obtained, suggesting higher temperature for single phase YIG. From VSM analysis, the average magnetic saturation, coercivity and remanence are 18.17 emu/g, 21.73 Oe and 2.38 emu/g, respectively. 1.0 wt% of YIG nanofluid was prepared and subsequently injected into the pre-saturated porous medium in the presence of square electromagnetic wave of 13.6 MHz. As much as 17.77%OOIP was recovered following to the injection of 2 pore volume of YIG nanofluid. In conclusion, magnetic nanoparticles is potentially being used for future EOR method to overcome current industrial limitation.

[1] H. Soleimani, N. Yahya, N. R. A. Latiff, H. M. Zaid, B. Demiral and J. Amighian:J. Nano Research Vol. 26 (2014), p. 111
[2] P. Mcelfresh, M. Wood, and D. Ector, SPE International Oilfield Nanotechnology Conference.(2012).

VIP041
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Application of Nanotechnology for Enhanced Oil Recovery: A Review
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Nanotechnology has significant contributions on developing modern industries, such as electronics, biomedical, materials, manufacturing, and energy industry. The changes introduced by nanotechnology, have currently extended to several areas for oil and gas industry, namely exploration, drilling, production, refining and enhanced oil recovery (EOR). This study focuses on attraction to the worldwide attention of nanotechnology and how this method effects on oil breakthrough and improves EOR. This Study also implies that parameters such as rock types, crude oil types, nanoparticle types, concentrations, and sizes, have significant factors on recovery factor through improving key-parameters such as oil relative permeability, interfacial tension (IFT), wettability, transmissibility and particles retention.

Key worlds: Nanotechnology, Nanoparticles, EOR, Recovery Factor, IFT, Wettability

DSL319
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Mass Transfer Behaviour in Hybrid Solvent Oil Recovery Processes
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The mechanisms of mass transfer in thermal solvent enhanced oil recovery processes and the influence of grid size in the numerical simulation of these processes is not well understood [1]. The literature has indicated that, experimentally, solvent fronts progress more rapidly that what can be predicted using current approximations. It has also been shown that under certain modelling conditions with coarser grid meshes, the influence of numerical errors can be substantial. The equations that govern thermal multiphase flow through porous media are extremely complex and it is very difficult to decouple the contribution of the mass transfer mechanisms from the thermal effects. This paper was written to increase the understanding of the mass transfer mechanisms in hybrid thermal solvent recovery processes through a detailed examination of the linear one dimensional advection diffusion/dispersion (ADD) equation. This equation was modeled using finite difference methods.

The effects of grid size were examined, as well as the influence of the parameters that govern the mass transfer mechanisms. In particular, a range of values for diffusion and dispersion coefficients as well as advection velocity were selected and applied in various numerical configurations to assess the impact of each of the mechanisms and their contribution to the movement of the solvent front. The parameters chosen for this study were based on experimentally estimated values for advection velocity, diffusion and dispersion coefficients. This study has indicated that all three mechanisms (advection, diffusion and dispersion) must be included to have the solvent front progress at rates that are consistent with experimental solvent front advance rates published in the literature to date [1]. This result suggests that diffusion alone cannot account for the movement of the solvent front with the range of values that have been studied.

[1] N. Edmunds,SPE Edmunds Neil R., 2013. "Observations on the Mechanism of Solvent-Additive SAGD Processes". SPE Paper 165419 presented at the SPE Heavy Oil Conference Canada held in Calgary, Alberta, Canada, 11-13 June.

Special Session 13
SURFACE TREATMENTS OF ADVANCED MATERIALS (SS13)

DSL257
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Influence of Thermal Annealing on the Structure and Mechanical Properties Coatings based on (Ti, Hf, Nb, Si)N

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Using the CAVE Cathode Arc Vacuum Evaporation (CAVE), nano-structured hard and super-hard coatings based on (Ti, Hf, Nb, Si)N of 1μm to 2μm thickness were manufactured. The coatings were studied using the proton micro-beam μ-PIXE, RBS, SEM with EDS, XRD, and tested for adhesion resistance, wear, and nano-hardness. It was found that a concentration of Ti, Hf, Si, and Nb metals as well as a bias potential applied to a substrate and residual pressure in a chamber (N or Ar/N) affected the formation regularities of solid solutions and quasi-amorphous phases based on α-Si3N4. Hardness of the resulting coatings reached 41.8 GPa. The friction coefficient was 0.12 to 0.45, and temperature resistance was as high as 900 oC.
The average size of the crystallites are exposed to the increase throughout the all temperature range of annealing and reaches maximum size of 7.7 nm at 1000°C, increases for more than 60% compared to the initial state.

[1]. A.D. Pogrebnjak, A.P. Shpak, V.M. Beresnev, D.A. Kolesnikov, Yu.A. Kunitsky, O.V. Sobol, V.V. Uglov, F.F. Komarov, A.P. Shypylenko, A.A. Demyanenko, V.S. Baidak, V.V. Grudnitskii, J. Nanosci. Nanotechnol. 12, 9213 (2012).
[2]. J. Musil, J. Vicek, P. Zeman, Adv. Appl. Ceram. 107, 148 (2008)

DSL272
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Nitriding Behavior of Ti6Al4V Alloy in Gas Atmosphere

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Samples of Ti6Al4V were treated by gas nitriding in α-Ti and β-Ti field. Gas nitriding provided formation of TiN layer with a nitrogen diffusion zone beneath it. In the scope of the present study, after structural characterization of the nitrogen exposed surfaces, dry sliding wear tests were conducted. The sample nitrided in α-Ti field exhibited better wear resistance along with a lower coefficient of friction against alumina ball under dry sliding conditions when compared to the sample nitrided in β-Ti field.

Key word: nitride, diffusion, Ti6Al4V, LOM, wear

DSL287
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Thermal Diffusion Processing for the Hard Boriding Surface Engineering for Wear- and Corrosion-Resistance Applications
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Engineering components, e.g. tubing systems for down-hole applications in oil and gas industry, slurry pump components, gears, turbine components for power generation and some other large size complex-shape components made of steels and alloys, require protection against sliding abrasion, friction, impact and corrosion. As one of the surface engineering solutions, CVD coatings consisted of the borides obtained through thermal diffusion of boron into the metallic base of the components may be used. The fundamental principles of the thermal diffusion process are formulated and outlined for the boriding. In opposed to the "conventional" CVD process, the thermal diffusion process does not require a complicated system of the insertion of reactive gases; the boron-reach gaseous species are formed due to high temperature reactions in the specially formulated powder mixes with consequent deposition and diffusion of boron into the substrate. Thermal diffusion process and quality of the coatings are defined by the batch composition providing the boron deposition and diffusion, temperature and time of the process, type of the metallic base and its surface quality and engineering design of the thermal diffusion CVD process system. The obtained hard boride coatings with crystalline structures with thicknesses of 50-250 up to 400 µm (depending on the metallic substrate and application) are uniform through the entire length of the components, do not have delamination issues, and they are successfully used in industry. The wear and corrosion extensive test results, as well as the structural features affecting the application properties, in particular, for the heavy oil production, are discussed. Superior application properties and integrity of the coatings are defined by high thermodynamic properties of the forming metal borides and strong covalent bonds B-B and Me-B, the diffusion-related bonding of metal borides with the metallic substrates (e.g. iron borides forming on conventional carbon steels have a "saw-tooth" structure), their high hardness (about 10 times higher than of untreated substrates). The boride-based coatings are successfully produced onto large-size and complex-shape industrial components, e.g. tubing and casing with length up to 12 m with the inner or inner and outer surface protection, and this technical solution provides significant extension of the component service life (typically from 3 to 10 times depending on the service conditions) in harsh wear-corrosion environments.

DSL293
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Effect of Severe Shot Peening on the Plasma Nitriding of Biomedical Ti6Al4V Alloy
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In this study, biomedical Ti6Al4V alloy has been subjected to plasma nitriding subsequent to severe shot peening. Severe shot peening exposes to the material high plastic deformation and forms dislocation densed nanograin layer. XRD and FESEM investigations show the nanograin layer possess grain sizes below 30 nm and the thickness emerges up to 60 µm according to the plastic deformation rate. Plasma nitriding has been performed to as received and shot peened specimens at 500, 550 and 6000C with the durations of 4h, 8h and 16h. XRD studies

show the TiN and Ti2N phase formations depending upon the nitriding temperature. The nitrogen diffusion zone has been increased by the raising of nitriding duration and temperature. Moreover, the diffusion zone has been influenced from severe plastic deformation via severe shot peening and increased up to 1.5 times when compared to only nitrided ones. The situation can be expressed by the beneficial effect of the highly dislocation and grain boundary densed nanostructured layer. The structure takes an active role as open channels for the diffusion of nitrogen atoms through interior.

DSL294
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Fatigue Behaviour of Biomedical Ti6Al4V Alloy subjected to Conventional Shot Peening Severe Shot Peening and Repeening

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Fatigue characteristics of biomedical Ti alloys particularly used in arthrosis surgery have been investigated due to in vivo dynamic load conditions. Shot peening is mainly used for improving fatigue properties of metallic materials. Severe shot peening (new type of shot peening) has been performed to biomedial Ti6Al4V create nano grained layer on the surface by means of severe plastic deformation in this study. Optical and FESEM studies show that dislocation densed nanocrystalline layer has been emerged after severe shot peening. XRD studies reveals severely deformed highly densed surface layer has nano grain size below 30 nm. Nano grain formation on the surface provides quite better mechanical and microstructural properties. The microhardness of the surface enhances at least two times with compared to as received ones. However, rotating bending fatigue tests show the fatigue limit raises slightly according to conventional shot peening due to disadvantage of surface roughness abrupt rise. Repeening application has been performed due to reduction of the surface roughness to reasonable values. Repeening leads to the surface roughness decrease and provides remarkable fatigue limit enhancement.

DSL304
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Growth rate of DyNi2 Film by Molten Salt Electrolysis

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Concerning the growth rate of YNi2 film, Xie et al. reported that the diffusion coefficient of Y in a single YNi2 phase region was estimated to be   cm2 s-1 by an electrochemical transient technique [1, 2]. Hachiya and Ito reported that the rapid growth is mainly due to the high-rate self-diffusion in and near the grain-boundaries by utilizing the molecular dynamics simulation [3]. Concerning DyNi2 and YNi2, a common mechanism which accounts for the rapid growth seem to exist because of same crystal structures, i.e., cubic Laves phase. From this background, kinetics of DyNi2 film growth by molten salt electrolysis was investigated in LiCl-KCl-DyCl3 (0.50 mol%) melts at 700 K. The rapid formation of a DyNi2 film, about 60 mm for 2 hours, was confirmed, in spite of such a low

experimental temperature as 700 K which is the half of melting point [4]. Furthermore, the growth rate depends on the applied potential, i.e., higher growth rate at more negative potential.

In this study, the formation of DyNi2 films was investigated at various potential and temperature. Thickness of each DyNi2 film was measured by cross-sectional SEM observation to estimate the growth rate of DyNi2 film. From the obtained information, the mechanism model of DyNi2 film growth was proposed.

[1] G. Xie, K. Ema, and Y. Ito, J. Appl. Electrochem., 23, 753 (1993).
[2] G. Xie, K. Ema, and Y. Ito, J. Appl. Electrochem., 24, 321 (1994).
[3] K. Hachiya and Y. Ito, J. Alloys Comp., 279, 171 (1998).
[4] H. Konishi, T. Nohira and Y. Ito, J. Electrochem. Soc., 148, C506 (2001).

DSL313
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Formation Kinetics and Properties of a Lower-Al Containing Aluminide Surface Layer on Ferritic-Martensitic Steel with a Gradient Nanostructured Surface Layer

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Ferritic-martensitic (F-M) steels are widely used in ultra-supercritical power plants. Aluminizing might significantly improve their oxidation resistance, and therefore elevate steam temperatures in service. However, conventional aluminization processes require high temperatures and induce serious deterioration in mechanical properties. While aluminizing temperatures are below the final tempering temperature (~775 °C) of F-M steels, the formed aluminide layer might not only be rather thin, but also be composed of brittle Al-rich aluminides.

In the present work, a gradient nanostructured surface layer was fabricated on a P92 F-M steel by means of surface mechanical attrition treatment (SMAT). The mean grain size is ~8 nm at the topmost surface layer and increases with depth. The aluminizing behaviors of the SMAT sample were investigated at temperatures around 700 °C. In comparison with the initial sample, a much thicker Al5Fe2 layer is formed on the SMAT sample, and the transformation kinetics from Al5Fe2 phase into AlFe and a-(FeAl) are also enhanced significantly. The enhanced aluminizing kinetics originate from the increased atomic diffusivities by numerous grain boundaries and a higher concentration of vacancies in the nanostructured surface layer.

Accordingly, formation kinetics of different aluminide layers have been determined on the SMAT sample. And a lower-Al containing aluminide surface layer of ~17 mm in thickness was produced following a duplex aluminizing process, including a packed aluminization process and a subsequent diffusion annealing treatment at lower temperatures. Experimental results showed that such an aluminide layer possesses high oxidation-resistance in steam at higher temperatures. Meanwhile, it is more resistant to cracking and has better adhesion to the substrate than the Al5Fe2 layer.

DSL333
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Development of Porosity in Thin Layers of Materials by the Implantation of Inert Gas Ions

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Gaining knowledge about damaging of cultural heritage objects is closely related with study of materials damaged by radiation fluxes and other acting factors present in the enviroment. Interaction gases with a lattice of material lead to degradation of its physical and mechanical characteristics, and can possibly generate flaws for new radiation-resistant materials, namely, for silicon carbide. Voids in lattice of 3C-SiC and clusters of gaseous nanobubbles investigated on theoretical grounds represent defects that can be studied by means of computer experiments. The simulation was performed using a kinetic theory, the model of Brownian motion of bubbles, and the stochastic simulation method [1]. The advantages of this approach are a rigorous mathematical framework, the quasi-linearity of the equations, and the unsteady character of nucleation consistent with a pulsed action on the blistering processes.

The condensation model of the liquid drops [2] considered as a phase transition of 1-st kind at initial stage, is conceptually identical to the nucleation model of gaseous bubbles in lattice due to penetration of Xe++ high-energy ions. Differently from the equilibrium stage where phase transitions of homogeneous nucleation are thermodynamically well-described and sizes of bubbles grow with constant rate, the presence of a significant amount of interfaces (grain boundaries and triple joints), which work as drain for the removal of radiation defects, can lead to a quality change of nanomaterials compared with coarse equilibrium predictions. Computer experiments are so related to non-equilibrium phase transitions in nano-objects, such as diffusion transport in gaseous pores. Therefore, the investigation of initial state porosity due to fluctuation of thermodynamical parameters of the system led to more easy penetration for pollutants as well as degradation of its qualities; these results are useful to define the initial and boundary conditions for a set of equations for degradation in buildings' materials. Analogous numerical approaches and algorithms will be used to solve the system of equations describing the time evolution of degradation on the surface and in the bulk of stones of historical buildings for comparison's sake with experimental measurements [3] (Infrared Passive Thermography, Scanning Electron Microscopy and Nuclear Magnetic Resonance). In future, the porosity resulting from computer experiments has to be compared with these three complementary experimental methods acting on samples with various pore-size scales (from mm up to nm) in objects of architecture and paintings.

[1] G.I. Zmievskaya, A.L. Bondareva, V.D. Levchenko and T.V. Levchenko, J. Phys. D: Appl. Phys. 40 (2007) 4842-4849.
[2] A.L. Bondareva, T.V. Levchenko and G.I. Zmievskaya, D&D Forum.V. 297–301: Diffusion in Solids and Liquids V: Trans Tech Publications.Switzerland (2010) 502-507.
[3] S. Bruni, M. Indirli, G. Maino et al., EAI Speciale II - 2012 Knowledge, Diagnostics and Preservation of Cultural Heritage (2012) 135-140.

DSL341
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Comparative Study of Corrosion Rate of Nickel-Titanium Alloy Surface Treated with Irradiation by Laser Beam for Application in Cardiovascular Stents

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Nickel-Titanium alloys have been extensively used in several branches of engineering and medicine, account of its properties such as the shape-memory effect, superelasticity and corrosion resistance, proving to be a revolution for science [1].This work, was applied the electrochemical technique of linear polarization, according the standard ASTM G3-89, 2004 [2], to obtain the corrosion rate of nickel-titanium alloys with nominal compositions (% weight) of 54.85%Ni-45.15%Ti; 55.00%Ni-45.00%Ti and 55.90%Ni-44.1%Ti for application in production of cardiovascular stents. The reactive solution used in the corrosion tests was Hank's Balanced Solution (T = 37°C ± 1ºC e pH = 7.0). For alloys containing   54.85%Ni-45.15%Ti, the values obtained for the corrosion rate were 0.02969 mm per year, whereas for alloys containing   55.00%Ni-45.00%Ti and 55.90%Ni-44.1%Ti the values were 0.0115742 0 and 009338 mm per year, respectively. The results indicated that all the alloys have good corrosion resistance, however the alloy containing 55.90%Ni-44.1%Ti by presenting a lower corrosion rate is the one that will suffer less wear and therefore have great useful life.

[1] Corte, D.A.D. Electrochemical behavior of Ni-Ti alloys: Study and Applications. School of Engineering of UFRGS, Porto Alegre, Brazil, (2008).
[2] AMERICAN SOCIETY FOR TESTING AND MATERIALS. ASTM G3-89(2004) Standard Practice for Conventions Applicable to Electrochemical Measurements in Corrosion Testing. Philadelphia, (2004).

DSL396
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Role of Si Solute Concentration on the Corrosion Resistance of Fe-20Cr-xSi alloy
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In this study, the effets of Si solution concentration on the general and localized corrosion behavior of Fe-20Cr-xSi stainless steels were examined. Different electrochemical techniques such as potentiodynamic poalrization (PD), linear polarization resistance (LPR), electrochemical noise analysis (ENA) were used for the investigations. Alloy compositions were especially designed to single out the effect of Si in Fe-20Cr ferritic stainless steels. The alloys were prepared in a vacuum arc melting furnace. The buttons were subsequently solution annelaed to homogenise the microstructure. It was found that with an increase in Si content of the alloys, corrosion resistance properties measured in terms of localisez corrosion resistance, critical anodic current desnity, metastable pitting density and passive film stability were all improved significantly.

Keywords: Stainless steels; Passive film; Silicon; Corrosion, Stainless steel

DSL402
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Isothermal and Cyclic Oxidation of the Ti-6Al-4V Alloy
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Titanium alloys contain α and/or β stabilizing elements in various proportions, depending on their application and mechanical properties. Among them, the Ti-6Al-4V alloy, which consisted of the (α+β) structure, is the most widely used due to its high specific strength, good corrosion resistance, and metallurgical stability [1-3]. In this study, the Ti-6Al-4V alloy was isothermally and cyclically oxidized at 800oC for 40 hours in air, and its oxidation behavior was characterized in terms of its oxidation rate, scaling rate, and scale spallation tendency. The isothermal oxidation tests indicated that Ti-6Al-4V oxidized fast and almost linearly, forming thick oxide scales. However, the scales that formed during isothermal oxidation were adherent. The cyclic oxidation tests indicated that the scales that formed on Ti-6Al-4V were highly susceptible to spallation owing to the large growth stress arisen and the thermal stress imposed during thermal cyclings. The formed scales frequently delaminated into several pieces owing to the excessive stress aroused by the repetitive thermal shock. Particularly, excessive oxidation and heavy spallation occurred at the edge of Ti-6Al-4V during cyclic oxidation.

References
[1] D. Eylon, S. Fujishiro and P.J. Postans, F.H. Froes, J. Met., 36 (Nov.), 55 (1984).
[2] G. Lütjering, Mater. Sci. Eng., A 243, 32 (1998).
[3] R.R. Boyer, Mater. Sci. Eng., A 213, 103 (1996).

VIP020
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Diffusion of Oxygen in Ti-10Mo-xZr Alloys studied by Mechanical Spectroscopy
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Titanium alloys have been widely used as biomaterials, especially for orthopedic prostheses and dental implants. Titanium has replaced Co–Cr alloys and 316L stainless steel due to its excellent corrosion resistance, mechanical properties, and biocompatibility. The aim of the development of titanium alloys is to create materials with improved properties for use as implants that can be used for a long period of time [1]. Interstitial elements, as oxygen, for example, change strongly the mechanical properties of the material and mechanical spectroscopy measurements are a powerful tool in the study of the interaction of these elements with the metallic matrix or substitutional solutes, providing information on diffusion and concentration of interstitial elements [2]. Samples of Ti-10Mo-xZr (x = 0, 5, 10, 15, 20 e 25 wt%) alloys were prepared in arc-melting furnace with argon atmosphere. The ingots were hot-rolled and submitted to a homogenization heat treatment [3]. The microestructural analysis was performed using XRD and SEM. In this paper, the effect of oxygen on the anelastic properties of Ti-10Mo-xZr alloys was analysed, using mechanical spectroscopy measurements. The diffusion coefficients, pre-exponential factors and activation energies were calculated for oxygen in these alloys. (Financial support: Capes, CNPq, FAPESP and FUNDUNESP).

[1] Y. Li; C. Yang; H. Zhao; S. Qu; X. Li; Y. Li, Materials 7, 1709 (2014).
[2] H. Mehrer: Diffusion in Solids: Fundamentals, Methods, Materials, Diffusion-Controlled Processes (Spinger-Verlag, Berlin 2007).

[3] J.R.S. Martins Jr.; R.O. Araújo; T.A.G. Donato; V.E. Arana-Chavez; M.A.R. Buzalaf; C.R. Grandini Materials 7, 232 (2014).

DSL226
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Improving the Surface Quality by the Process of Vibratory Grinding

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The vibratory grinding is a method of treating chemical mechanical surface, which is to use the technology to low frequency vibration in the treatment of metal parts in the presence of abrasives and chemical additives. The treatment regimen and its parameters have a great influence on the geometric characteristics, mechanical and metallographic surfaces. The vibratory grinding process has many technical and economic advantages, especially for bulk processing of mechanical parts with complex shapes. In our present work we deal with several samples of different materials by the method of vibratory grinding in order to improve their surface states.

Keywords: roughness, hardening vibratory grinding, amplitude, frequency

DSL268
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Effect of the Vibro-Impact Process on Improving the Life of Mechanical Parts

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One of the most important tasks of modern engineering is to find ways to improve the quality, reliability and durability of the parts, by improving technological methods of hardening treatment. The quality of the surface state of the parts in contact of moving or stationary parts is essential for the reliability of use and improving their lifetime. The contact surface parts is then regarded as one of the functional parameters of surface quality. Thus, we used the vibro-impact treatment which improves the mechanical characteristics and allows smoothing the micro geometry and hardening of the surface layer. This treatment creates plastic deformation on the surface layer of the parts by inducing compressive residual stresses that cancel the effect of stress concentrators and thus increase the longevity of the treated parts. The objective of this study is to improve the performance of functional surfaces in contact through a judicious choice of optimum hardening parameters. This paper presents the effects of the process by vibro-impact on the fatigue strength of samples from steel, aluminum and bronze.

Keywords: Contact mechanics, hardness, fatigue, Surface treatment, residual stress.

References

[1] A.P. Babichev, I.A. Babichev: Principle of Vibration Technology, Rostov-sw-Don Russia, ISBN 978-5-7890-0472-2; 2008

[2] A.P. Babichev, P.D. Matrenko et al.: Finishing-hardening treatment details by multi- vibro impact-tool, Rostov on Don, DSTU, 2003, p. 191

[3] D.D. Ivlev, G.I.Bekovtcev: Theory of a hardening plastic body, M. Nauka, 1971.

DSL375
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Preparation and Structural Characterization of Ultrathin Polymer Films by Neutron Reflectivity

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Neodymium-iron-boron alloys are very sensitive, particularly to the air humidity. To protect against corrosion, the neodymium magnets are covered by a layer of nickel, nickel-copper or aluminum. The aim of our work is to study the effectiveness of polymer coatings against corrosion in the cases cited above. In this context we introduced the neutron reflectometry [1] to study the ultra-thin polymer film interfaces. All experiments were conducted at the nuclear research center of Draria (Algiers). The principle of the specular neutron reflection is to measure the reflection coefficient R of a neutron impact under small angle on the surface studied [2]. We use monochromatic long-wavelength neutrons and θ (reflection angle)-2θ (detector angle) scan. The reflectivity, R, depends on the scattering vector Q, defined by: $Q = 2\pi (\sin\theta)/\lambda$. First, we realized calibration settings "zero" reflectometer: one seeks the zero position of the detector, the optimal position of the sample and its angle of rotation. The elaboration of the films is carried out by a method known as the '' spin-coating''. This technique provides dense, homogeneous and very thin material. We have prepared a thin film of polymethyl methacrylate (PMMA) [3]. In a second step, we examined the polymer film by SEM and XRD. The micrographs show the presence of varying size bubbles and dark areas in contrast due to surface inhomogeneities. The spectrum shows the Kiessig interference fringes whose frequency allows us to determine the film thickness e=483nm and $\Delta Q=0.0013$ nm-1. The high background level did not allow us to achieve the convergence of the adjustment by the Parrat recurrent models [4]. To solve this problem we surrounded the detector with two screens, one in paraffin and other light water.

[1] Penfoldt J., Thomas R. K."The application of the specular reflection of neutrons to the study of surfaces and interfaces"J. Phys.: Condens. Matter 2, 1369-1412 (1990).

[2] Fermon C. Ott F. Menelle A. X-ray and neutron reflectivity: Principles and Applications. J.Daillant, A.Gibaud edition, 1999.

[3] Guedioura B., Bendjaballah N., Alioui N., "Profiling measurements of metal ion distribution in thin polymer inclusion membranes by Rutherford backscattering spectrometry", Radiation Effects and Defects in Solids, 169, 5, 2014, 388-395..doi.org/10.1080/104 20150.2013.865621.

[4] Parratt 32 by Chr. Braun, Hahn-Meitner-Institut Berlin, 1999.

DSL224
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Comparative Analysis of the Surface Roughness Parameters due to the Surface Machining Uniformity

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In the paper a new method has been proposed for determining of the very fine machining uniformity over the elaborated surface and could be applied to the different machined materials and machining pro¬ce¬du¬res. The proposed methodology is relatively simply and it's essential is formulated in the few sub¬se¬quent steps:
• taking surface roughness 3D profile accordingly proposed scheme – over the four apart mea-su¬re¬ment fields, with using AFM or optical profilometer, providing data as the set over square grid;
• estimation of the roughness statistical parameters: Rp, Rv, Rt, Ra, Rq, Rskew, Rkurt, and if need be – surface rugosity Ru; accordingly usual methodology;
• calculation of the centroid of the obtained data due to the measurement fields,
• calculation of the barycentre of the obtained data with the weighting variable chosen for the appro¬priate evaluation of the surface machining uniformity.
As the main Cartesian coordinates of the centroid calculation we propose (Rskew, Rkurt), although other data organization schemes have also been provided as the exemplary solutions. The final evaluation of the surface machining uniformity is based upon the Euclidean distance between centroid and barycentre of the surface roughness data. Zero distance means ideal machining uniformity. The proposed method has been applied to experimental results obtained with used AFM tech¬ni¬que on samples of the polished AZ31 magnesium alloy. The surface machining procedure comprised of four stages performed with using different abrasive media, finally lead to the highest grade of the surface roughness. The whole set of data has been taken after each stage, which allowed the very precise evaluation of the machining pro¬ce¬du¬re due to its roughness results as well as the machining uniformity over the surveyed surface area.
The main advantage of the proposed methods lays it's applicability to the data from the very different surface machining techniques, leading to the surface roughness statistical parameters differing in orders of magnitude, without affecting of its main goal – estimation of the surface machining uniformity.

DSL276
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Corrosion Monitoring of the Active / Passive / Transpassive State of a High-Alloy Crmnni-Steel by Acoustic Emission

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The electrochemical corrosion behaviour of an high-alloy steel, containing 16 wt.% Cr, 6 wt.% Mn and 3 wt.% Ni was electrochemically polarised in a 0.5 M sulphuric acid solution. In consideration of the characteristic regions of its active, passive and transpassive state, the steel was potentiostatically polarised and the acoustic emission signal was recorded simultaneously at a distance of 5 cm from the location of corrosion. The test had a duration of 180 s involving a measurement of acoustic emission for 30 s at the open circuit potential, 120 s at applied potential and 30 s at open circuit potential after polarisation. Furthermore, as a reference the acoustic emission was recorded for 180 s without polarisation. The analysis of the acoustic emission signals revealed an increase of corrosion events when the steel was cathodically polarised whereas a significant reduction in intensity is observed

when the material is anodically polarised. In comparison to the unpolarised electrode the acoustic emission signal exhibits a continuous decline when the steel is polarised into the active / passive state whereas a sharp point of inflexion is recognized when the applied potential causes a spontaneous passivation. Moreover, the signal intensity increases again when the transpassive state is reached, which revealed a further increase of electrode activity. All acoustic emission signals were related to a blistering at the steel / electrolyte interface. The high signal intensity at cathodic polarisation is associated with an intensified hydrogen formation. Furthermore, when the steel is anodically polarised, the continuous decline at the active / passive state reveals the time for passivation of the material. In contrast, when the applied potential reaches the passive state, the acoustic emission signal is reduced abruptly indicating the hindrance of anodic dissolution due to passivation. At starting transpassivity the acoustic emission signal shows lowest intensity. However, in contrast to lower applied anodic potentials, an increase of acoustic emission is observed due to the onset of oxygen evolution at the steel / electrolyte interface.

DSL289
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Isothermal and Cyclic Oxidation of Ti-6Al-4V Alloy

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Titanium alloys contain α and/or β stabilizing elements in various proportions, depending on their application and mechanical properties. Among them, the Ti-6Al-4V alloy (hereafter termed as Ti64), which consisted of an (α+β) structure, is the most widely used due to its high specific strength, good corrosion resistance, and metallurgical stability [1,2]. The isothermal oxidation of Ti64 followed the parabolic kinetics between 600 and 700ºC and linear kinetics above 700ºC, while the surfaces were mainly covered with anatase- and rutile-TiO_2.The cyclic oxidation is as important as the isothermal oxidation, because alloys frequently experience thermal shock during their service, resulting in cracking and spalling of the scales. Hence, the isothermal and cyclic oxidation behavior of the pure Ti metal and the Ti64 alloy was studied at 600-800ºC in air, and the oxidation kinetics, and the properties of the oxide scales are described in this study. The Ti-6Al-4V alloy was oxidized isothermally and cyclically in air, and its oxidation behavior was compared with that of the Ti metal. The isothermal oxidation at 800°C indicated that Ti-6Al-4V and Ti oxidized fast almost linearly, and the oxide scales that formed on Ti-6Al-4V and Ti were nonadherent. The cyclic oxidation indicated that Ti-6Al-4V oxidized faster than Ti at 600°C, and serious scale spallation occurred in Ti-6Al-4V compared to Ti at 800°C. The oxide scales that formed on Ti-6Al-4V and Ti after cyclic oxidation at 800°C delaminated into several pieces owing to excessive stress aroused by the repetitive thermal shock.

[1] C.R. Brooks, American Society for Metals, USA, 330 (1982).
[2] W.F. Smith, Structure and Properties of Engineering Alloys, McGraw-Hill Book Co., New York, 438 (1981).

DSL290
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Plasmon-Induced Efficiency Enhancement on Dye-Sensitized Solar Cell by a 3D TNW-Au NP Layer

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AR films with light trapping characteristics played a pivotal role in enhancing the efficiency of photovoltaic devices. For Si photovoltaic devices, surface textured AR coatings with porosity and roughness could take advantage of light trapping to increase the absorbance. For thin-film devices, AR films generally consist of more dielectric layers to improve light trapping performance, giving a more broadband response in reflection. In the on-going single-layer AR coating revolution, we previously had been successfully utilized a low-temperature (80 oC) method on the growth of a single-layer (~600 nm) of TiO_2 NWs onto fluorine tin oxide (FTO) substrates.[1] In this work, a new 3D TNW-Au NP plasmonic electrode consists of antireflective (AR) TiO_2 nanowires (TNWs) (~600 nm thickness) serving as light-harvesting antennae coupling with Au nanoparticles (NPs). A huge redshift of 55 nm is observed in surface plasmon spectra for the Au (11 nm) plasmonic electrode that has 11 nm size Au NPs, whereby (111) lattice planes have a specific bonding with the TiO_2 (101) planes. Remarkable redshift is mainly attributed the localized electric field improvement resulting from the plasmonic coupling effect between the Au NPs and the Au-TiO_2 hybrids. After $TiCl_4$ treatment, this favorable Au (11 nm) nanostructure takes advantage of harvesting photons to increase the conversion efficiency of DSSCs from 6.25 % to 9.37 %.

1. Chen, J.-Z.; Ko, W.-Y.; Yen, Y.-C.; Chen, P.-H.; Lin, K.-J., Hydrothermally Processed TiO_2 Nanowire Electrodes with Antireflective and Electrochromic Properties. ACS Nano 2012, 6, 6633-6639.

DSL291
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Formation and Characterization of Hard Coatings on Ductile Iron Grade 100-70-30

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This paper studies the formation of iron boride on the surface of a ductile iron 100-70-03 class exposed to thermochemical treatment boron dehydrated paste. The formation of iron boride layers Fe_2B FeB-type, were obtained at temperatures of 900ºC, 950°C and 1000ºC, with exposure times of 8 hours of treatment. The study consisted in evaluating the growth kinetics of the boride layer on the surface of ductile iron boriding. Also the boride layers were determined by the XRD method, EDS. Also evaluated fracture toughness technique Vickers microindentation 15 and 30 microns from the surface with different loadings of iron boride microindentation formed on the surface.

[1]Yusuf Kayali, Sukru Taktak, Sinan Ulu, Yilmaz Yalcin, Mater and Design 31, 1799–1803 (2010)
[2] Ugur Sen, Saduman Sen, Fevzi Yilmaz, Jour of Mater Proc Techno 148 1–7 (2004)
[3] Ugur Sen, Saduman Sen, Sakip Koksal, Fevzi Yilmaz, Mater and Design 26 175–179 (2005)
[4] Murat Baydoga, Seckin Izzet Akray, Jour of Iron and Steel Resear. Interna. 16(2), 50-54 (2009)

[5] Fatma Ünal and Ahmet Topuz, Materials Testing 56, 6, 483-485 (2014)

[6] N. López Perrusquia, M. A. Doñu Ruiz, E. Y. Vargas Oliva and V. Cortez Suarez. MRS Proceedings, 1481, 105-112 (2012).

[7] N López Perrusquia, M A Doñu Ruiz, D Sánchez Huitron, J. D. Villegas Cárdenas, A. Camarillo Villegas, IOP Conf. Series: Mater Scien and Engin, 45, 1-4 (2013)

DSL295
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Modelling of Composition and Stress Profiles in Low Temperature Surface Engineering
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Thermochemical surface engineering by nitriding/carburizing of stainless steel causes a wear and corrosion resistant case of expanded austenite. As a consequence of the thermochemical surface engineering, huge residual stresses are introduced into the case, arising from the volume expansion that accompanies the dissolution of high contents of nitrogen/carbon in austenite.

Modelling of the composition and stress profiles developing during low temperature surface engineering from the processing parameters. A realistic model should take the following into account:

- concentration dependent diffusion coefficient
- finite flux of interstitials through the surface
- trapping of nitrogen/carbon
- effect of residual stress on diffusive flux
- effect of residual stress on solubility of interstitials
- plastic accommodation of stress exceeding the yield strength

The effect of all these contributions on composition and stress profiles will be addressed and the differences between nitriding and carburizing will be discussed.

DSL308
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Electromigration Experiments in the Ag-Zn System by Spark Plasma Sintering
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This study reports on experiments of electromigration during reaction in Ag-Zn diffusion couples annealed in a spark plasma sintering (SPS) apparatus. The aim is to investigate fundamentally the role of the high electric current pulses involved in this technique in accelerating diffusion processes occurring during reaction.

The SPS is a hot pressing system, in which punches apply a uniaxial pressure on powder samples and simultaneously a pulsed current which heats up the sample and its surrounding graphite matrix by Joule effect. The very fast sintering rates achieved by this technique have been interpreted by the influence of the electric pulses on the sintering phenomena, as creation of arcs and plasma between the powder particles, or acceleration of metallurgical phenomena (diffusion, plastic deformation…). Here, we address fundamentally the question of acceleration of diffusion kinetics by the electric current of the SPS (electromigration). For this purpose, instead of powder samples, diffusion couples of the Ag-Zn system, which is reported to be sensitive to electromigration [1], have been introduced in the SPS, and annealed at 300°C for 2 to 20 min. Sample preparation and control of temperature profile proved to be determinant for properly carrying out the experiments. The kinetics has been measured by following the evolution of the thickness of the intermetallic product layer forming at the interface between Ag and Zn. The experiments have been performed with the SPS current ($J = 50\text{-}200$ A/cm2), but also with dedicated experimental setups in which the samples were insulated from the current ($J = 0$ A/cm2), or on the contrary in which the current was artificially increased ($J = 1000\text{-}1400$ A/cm2). With $J = 0$ A/cm2, the kinetics was parabolic in time and hence controlled by diffusion. This kinetics was not modified in the presence of the current up to $J = 1000\text{-}1400$ A/cm2, meaning that no electromigration phenomena occurred.

[1] J.R. Friedman, J.E. Garay, U. Anselmi-Tamburini and Z.A. Munir, Intermetallics, 12, 589, (2004).

DSL309
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Oxidation of Hot Extruded AZ31 Magnesium Alloys Containing Initially Added CaO Particles
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Particles of (0.5, 1, 1.5)wt.%CaO were added during casting into the AZ31 magnesium alloy having a nominal composition of Mg-3%Al-1%Zn in wt.%, and hot extruded to a plate having a thickness of 2 mm. The CaO-added AZ31 magnesium alloy plate was oxidized between 450 and 650oC in atmospheric air in order to find the effect of the initially added CaO and hot extrusion on the oxidation of Mg alloys. Initially added CaO particles reacted with the AZ31 melt, and precipitated as Al_2Ca particles along the grain boundaries of the AZ31 alloy during casting. The Al_2Ca particles increased the oxidation resistance of the AZ31 alloy. The more the Al_2Ca particles were, the better the oxidation resistance of the AZ31 alloy was. During oxidation, the MgO oxide scale that incorporated with CaO formed at the surface of the AZ31 alloy.

DSL316
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Characterization and Fracture Toughness on AISI 8620 with Hard Coatings
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The present studies characterize and evaluate the fracture toughness at the surface AISI 8620 with hard coating. The hard coatings FeB and Fe2B were formed using the boriding dehydrated paste for at temperatures 1223 and 1273 K with 6 and 8 h exposure time, respectively. The presence of hard coating formed on the surface AISI 8620 were confirmed by classical metallographic technique combined with X-ray diffraction analysis. The distribution of alloying elements was determined by energy dispersive Spectroscopy (EDS).

The fracture toughness of the hard coatings on AISI 8620 was estimated using a Vicker microindentation induced fracture testing of 15 and 35 µm from the surface, applying four load (0.49, 0.98,1.96 and N). The microcrack generated at the corner of the microindentation was considered as experimental parameters and tree model Palmqvist crack model were employed to determine the fracture toughness [1].

The adherence of the hard coatings/substrate was evaluate in qualitative form though the VDI 3198 [2] by testing Rockwell C and observed by scanning electron microscopy. SEM. The formation of hard layers was obtained in the range of 100-130 µm, results of XRD present phases FeB, Fe2B, CrB and MnB, the values obtained of Kc are in the range of 2.3 to 4.9 MPam½ and results of acceptable adhesion HF4 patterns for conditions 6 h of treatment.

[1] D. K. Shetty, I. G. Wright, P. N. Mincer, A. H. Clauer. Journal of Materials Science 20 (1985) 1873-1882.
[2] Vidakis, N., Antoniadis, A., & Bilalis, N. J. Mater. Process. Technol., 2003, 143-144, p 481-485.

DSL317
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High-temperature Oxidation Behavior of High Strength Steels

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Since it is important to reduce the weight and increase the crashworthiness of cars, steel plates with high strength became necessary. Hence, steel mills are producing high strength steel plates using their own distinctive procedure. In this study, the oxidation behavior of three kinds of high strength steel plates, which were produced by three different steel mills, were studied in order to find the difference in the oxidation behavior. The three steel plates were oxidized at 900oC in atmospheric air isothermally and cyclically, then their oxidation characteristics were compared. The composition of the steels significantly affected the scaling rates, the composition, thickness, and adherence of the formed scales. The most important element in term of oxidation was Si, which can form extremely slow growing SiO2 on the surface, but can decrease the scale adherence. Steel plates with a low Si concentration oxidized fast, forming thick scales with poor adherence, while steel plates with a high Si concentration oxidized slowly, forming thin scales with poor adherence. Si oxidized to SiO2, which further reacted with iron oxides to form a thin protective Fe2SiO4 layer at the scale-metal interface, which blocked the diffusion of ions thereby to reduce the oxidation rate.

DSL347
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An Effective Way to Increase Threshold Current Density against Electromigration of a Metal Line
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Enhancement of electromigration (EM) reliability for electronic devices composed of metal lines is important for improving those lifetime [1]. Electromigration causes harmful damages which are voids and hillocks in a metal line because of the diffusion of metallic atoms with high density electron flow. The threshold current density is a measure for improving EM reliability. The threshold current density is defined as the critical value of current density by which the voids and hillocks begin to form in a passivated metal line [2]. The EM reliability can be improved by increase of the threshold current density, and many researchers have made efforts to increase it by various approaches. The formation of passivation onto a metal line and the decrease of substrate temperature are common ways to improve the EM reliability. The deposition of passivation is one of the countermeasures for preventing the EM damages because that inhibits the growth of voids and hillocks by covering a metal line [3]. The decrease of substrate temperature is positive approach for mitigation of EM because atomic diffusion caused by EM is subject to temperature. Therefore, the quantitative relation of the threshold current density with passivation thickness and substrate temperature is required. In the present study, we demonstrate an effective way to increase the threshold current density through experiments for samples with different passivation thickness and different substrate temperature. The threshold current density is shown to be increased by forming the passivation with appropriate thickness and decreasing substrate temperature into an appropriate range. This work was supported by JSPS KAKENHI Grant-in-Aid for Scientific Research (B) No. 26289001.

[1] C.M. Tan and A. Roy, Mater. Sci. Eng. R, 58, 1 (2007).
[2] I.A. Blech, J. Appl.Phys., 47, 1203 (1976).
[3] J.R. Lloyd, P.M. Smith and G.S. Prokop, Thin Solid Films, 93, 385 (1982).

DSL364
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New Insights into Sulfidation Reactions of Metal Oxides used as Sulfur Sorbents: Solid-State Transformation Mechanism and Kinetics Modelling
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Fischer-Tropsch (FT) based XTL processes and IGCC technologies are attractive alternatives for future energy production [1]. In order to prevent unit corrosion or FT catalysts poisoning, deep desulfurization of synthesis gases or natural gases is achieved with metal oxides, like zinc oxide, which reacts with H2S according to the reaction: $ZnO(s) + H_2S(g) \rightarrow ZnS(s) + H_2O(g)$ The use of metal oxides as sulfur sorbents allows to reach very low H2S levels in the treated gases, due to the highly favored sulfidation reactions. Although ZnO sulfidation reaction has also been widely studied [2], little is known about the transformation into ZnS at the crystal scale, its detailed mechanism and kinetics. In this communication, we will present last advances in this field. These results show

evidences for an outward growth process of the resulting ZnS phase, which are in contradiction with the previously admitted assumption of an inward growth on ZnS with diffusion of sulfur species [3]. Indeed, characterizations (e.g. TEM & electron tomography) of sulfided ZnO particles reveal voids formation resulting from Kirkendall effect. As a consequence, the diffusion step is more likely to involve a diffusion of zinc and oxygen atoms from the ZnO/ZnS internal interface to the outer surface of the ZnS particle. Related characterizations, reaction mechanism proposed, and related kinetics modelling will be presented [3]. More general questions arise from this work regarding the investigation of solid-state diffusion mechanisms involved in sulfidation reactions.

[1] D. Vallentin, Energ. Policy, 2008, 36(8), 3198; O. Shinada, A. Yamada, Y. Koyama, Energ. Convers. Manage., 2006, 43(9-12), 1221.
[2] A. Samokhvalov, B.J. Tatarchuk, PCCP, 2011, 13, 3197.
[3] L. Neveux et al., Chem. Eng. J., 2012, 181-182, 508; L. Neveux et al, PCCP, 2013, 15(5), 1532.

DSL369
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Optical Micro-Concentrator System for Enhancing Conversion Performances of Solar Cells
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In this paper, we present a new approach for an optical micro-concentrator system consisting of an array of microcavities on glass substrate and an intermediary layer of fluidic filler material , on the front surface of solar cells. The micro-concentrator system can therefore replace a conventional glass as a means of packaging of the cells to enhance photovoltaic performances of semiconductor based solar cells. The optical micro-concentrator on planar glass is fabricated using simple photolithography technique that make the design compatible with solar cell based on semiconductor technology and large-scale manufacturing. By covering the cell with micro-textured glass and an intermediate layer a hybrid optical system is obtained which improves the short-circuit photocurrent value.
We experimented a honeycomb texturization on Corning glass plate of 2x2 cm2 area. Wet etching process in KOH solution resulted led to obtaining a network of transparent micro-cavities of 20 μm diameter and a depth of 6 μm. The intermediary layer was chosen in function of refractive index, filler materials with refractive index in the range 1 - 1.43 were experimented. The structures of silicon solar cells covered with this optical micro-concentrator system were characterized by measuring the short-circuit photocurrent (open-circuit voltage being const.). An increase of 8% of the short-circuit photocurrent for the solar cells with optical micro-concentrator system compared with the a structure covered with an untextured glass was obtained. The simulations of this system were done by using OptiFTDT software. The aim of the simulations was to establish the optimum intermediary material regarding refractive by analysis of distribution of the radiation which cross the optical micro-concentrator system and reaches the surface of solar cell. The simulation results are in accordance with obtained experimental data for a filler material having n=1.43.

DSL372
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High Temperature Corrosion of Al Hot-dipped Low Carbon Steels in N2/H2S-mixed Gases
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A carbon steel whose chemical composition was Fe-0.04C-0.15Mn-0.02Si-0.012P-0.01S-0.05Cu-0.03Sn-0.006N in wt% was hot-dipped in the molten Al bath at 800oC, and corroded in N2/2.5%H2S-mixed gases at 650-850oC for 20-50 h in order to study its performance in the sulfur and hydrogen environment. The SEM/EDS and XRD techniques were used to study the elemental distribution, the morphology, and the corrosion mechanism. A thin Al topcoat and a thick Al5Fe2-rich layer containing a small amount of FeAl and Al3Fe formed on the surface after hot-dipping. Hot-dipping increased the microhardness of the steel by about 7 times. During corrosion, the decrement of microhardness through interdiffusion between coating and substrate occurred, internal voids formed in the intermetallic layer in Al hot-dipped steel, and the intermetallic Al5Fe2+Al2Fe+Al3Fe2 layer gradually transformed into the AlFe layer. The corrosion rate increased with an increase in temperature. After corrosion, the thin alumina layer that formed on the surface spalled. The uncoated carbon steel sulfurized to FeS through the outward diffusion of Fe ions from the matrix. FeS facilitated the growth of the underlying scale that consisted of FeO, Fe3O4 and Fe2O3. Al hot-dipping was found to increase the corrosion resistance of carbon steel through forming a thin protective α-Al2O3 scale in the outer layer.

Keywords: Carbon steel, Hot-dip aluminizing, microhardness, H2S corrosion.

DSL381
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Experimental Investigation and Modeling of Cracking Process of TBC in Critical Engine Parts
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Critical engine parts of aircraft engines such as blades and combustion chambers are exposed to high temperatures and corrosive environment during the operation time. Therefore, they are protected against the damage by Thermal Barrier Coatings (TBCs) made of several thin layers. The blades of turbine engines are additionally exposed to high mechanical loads. These loads are created by the high rotational speed of the rotor (30 000 rot/min), causing the tensile and bending stresses. Therefore, experimental testing of coated samples is necessary in order to determine strength properties of TBCs.
In the experimental program we used beam samples of dimensions 50x10x2 mm. TBC system consisted of 150mm thick bond coat (NiCoCrAlY) and 300 mm thick top coat (YSZ) made by APS (air plasma spray) process. The samples were subjected to 4-point bending test with various loads. After bending tests, the samples were subjected to microscopic observation to determine the quantity of cracks and their depth.
Obtained results were applied to formulate numerical model in ABAQUS code with experimental material. Brittle cracking damage model was applied for the TBC layer, which allows to remove elements after reaching criterion.

Surface based cohesive behavior was used to model the delamination which may occur at the boundary the between bond coat and the top coat.

Special Session 14
BIOMEDICAL IMPLANTS AND DEVICES (SS14)

DSL252
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Non Newtonians Fluid Flow Visualization Behavior using PIV Simulation Applied to a Tub Diffusion Convection

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Non Newtonians fluids became of great interest in Flow Visualization PIV (Particle Image Velocimetry), basically in Industry applications (Oil companies. Petrochemical, and chemical) in this millennium.. This work develops an image processing algorithm [1] which allows capture fluids in very low velocities, using a conventional camera in order of 10¬-1 cm/s. A cylindrical glass bench of 250 mm, permits the flow visualization. Water at temperature of 70 centigrade degrees, provides the convection for a PIV catch velocity and vorticity fields of vectors, and to another's lower temperatures. A analytical vortex model is developed to contrast to this experiment. Theses velocities turn possible studies of Non Newtonians fluids characteristics profiles of different test bench. Tubular pipes, planar on laminar flow, and others complex geometry can be studied given complete velocity field in real time at precision of PIV techniques. A visualization of 3D Vasenol foam precipitation is present in transparent green dynamic image.

[1] R. Pizzato, N. Caetano, F.T. van der Laan, Flow visualization of dynamics fields of velocity and vortex vectors program algorithm, Modern Mechanics Engineering, 2011

DSL366
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Computational Modelling of a Multi-Layered Biosensor with Diffusion Limiting Region

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Biosensors are analytical devices used for the detection and recognition of the chemical substances in solutions to be analysed. During the biosensor operation the substrate to be analysed is biochemically converted to a product. The signal is usually proportional to the concentration of the product. The mathematical model of the multi-layered biosensor with chemically modified electrode (CME) is analysed in this work [1]. The model (see [1], eq. (6)-(24)), described by non-linear reaction diffusion equations, involves three compartments: an enzyme layer, a dialysis membrane and a diffusion layer.

Selective membranes are commonly used to increase biosensors selectivity [2, 3]. Recently, a calculation of the biosensor based on Michaelis-Menten kinetics behaviour was conducted, taking into account the possibility to trap the signal formatting product by using similar membrane [4].

The purpose of this work was to investigate the influence of the product limiting region on the CME biosensor response and sensitivity. The original mathematical model of biosensor with CME was supplemented with a product trapping region and solved numerically by applying the Crank-Nicolson finite difference method [3]. The simulations showed that diffusion limiting membrane used for product trapping is a perspective way to optimize the behaviour of the CME biosensor at wide range of model parameter values.

[1] V. Ašeris, R. Baronas and K. Petrauskas, Comp. Appl. Math., Published online, DOI: 10.1007/s40314-014-0197-9 (2014).

[2] R. Baronas, J. Kulys and F. Ivanauskas, J. Math. Chem., 39, 345 (2006).

[3] R. Baronas, F. Ivanauskas and J. Kulys, p.334. Mathematical Modeling of Biosensors (Springer, Dordrecht, 2010).

[4] F. Ivanauskas, P. Katauskis and V. Laurinavičius, J. Math. Chem., 52, 689 (2013).

DSL403

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Electrostatic Nano-Stitches for DNA: Atomistic Simulations of Ca-Mediated Adsorption of DNA on Phospholipid Membranes

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Formation of supramolecular complexes of DNA and zwitterionic phospholipids is important from the point of view of the development of non-toxic gene delivery vectors and DNA-based nanodevices interacting with cell membranes. While experimental studies have shown that divalent cations can promote adsorption of negatively charged double helixes of DNA on zwitterionic (neutral) phospholipid membranes, the underlying molecular mechanism of such adsorption as well as the microscopic structure of the resulting supramolecular DNA-membrane complexes are still unknown. To address this problem, here we employ atomic-scale molecular dynamics simulations to probe interactions between DNA and phospholipid bilayer membranes in aqueous solution with and without $CaCl_2$ salt. The state-of-the-art atomistic force-fields AMBER parmbsc0 and AMBER Lipid14 were used to describe a double helix of DNA and phospholipid molecules, respectively. We carried out microsecond-long molecular dynamics simulations which allowed us to evaluate a wide range of dynamic and structural characteristics of DNA-membrane systems. Overall, our results provide compelling evidence that Ca ions are largely responsible for attractive interactions between DNA and phospholipid membranes on a nanoscale: We demonstrate that divalent calcium cations serve as nano-stitches between phosphate groups of DNA and lipid molecules, stabilizing thereby DNA-lipid complexes.

DSL406

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Use of Pseudoboehmite Nanoparticles for Drug Delivery System of Glucantime®

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The incidence of American Cutaneous Leishmaniasis (ACL) has, in recent years, growing in Latin America, especially Brazil, where from 1980 to 2005 605,062 cases were recorded. The drug Glucantime ® whose active principle is the meglumine antimoniate (or meglumine antimonate), is used in the treatment of leishmaniasis, its toxicity is due mainly to the presence of antimony in its structure, thereby determining the control of the doses as an essential factor in the treatment. Drug delivery systems are currently the focus of many studies before its effectiveness in treating disease and favorable performance compared to conventional methods. Due to some advantages, they can avoid repeated doses, also the substantial decrease the amount of drug intake, which not only enhance the therapeutic effect, but also reduces the risks of plasma concentration reaches toxic levels. Synthetic nanomaterials have attracted great interest for applications in pharmaceutical technology focused, so that control of their size and composition allows the best performance in interaction with the drug and its release. Pseudoboehmite is a synthetic aluminum compound precursor of alumina[1], with the same structure of boehmite and active groups in their structure[2], which characterizes it as an excellent adsorbent material. In the present work, pseudoboehmite prepared by sol-gel process for use as an excipient. The incorporation of pseudoboehmite in Glucantime® performed in the processing of tablets. The tablets were characterized by nitrogen adsorption isotherm, X-ray diffraction (XRD), Differential thermal analysis, thermogravimetry analysis (TG), Scanning Electron Microscopy (SEM) using secondary electron detector and EDS detector. The release profile obtained by UV/Vis spectroscopy for in vitro simulation. The results showed that there was no reaction between the drug and excipient.

[1] A. H. MUNHOZ et alii The Influence of Ageing in Pseudoboehmites Synthesis. Materials Science Forum (Online), v. 727-728, p. 1795-1801, 2012.
[2] E.M. moroz et alii. Local structure of pseudoboehmites, React.Kinet.Catal.Lett, Vol. 87, No. 2, 367-375, (2006)

DSL412
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Drug Transport in Charged Polymeric Hydrogels for Drug Delivery
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The ability to provide tunable drug delivery rates represents one of the most promising medical approaches of the last years. In this framework, hydrogels are widely investigated polymeric scaffolds due to their ability to mimic living tissues together with their high biocompatibility. Here the interpretation of transport phenomena is a key step, but nevertheless within these systems is still controversial and a comprehensive theory lacks [1,2]. We investigated a promising agarcarbomer (AC) hydrogel library loaded with ethosuximide (ESM), an anticonvulsant drug. The self-diffusion coefficient of ESM in AC formulations was measured using two methods: a direct measurement with pulsed field gradient spin-echo (PFGSE) method, using an NMR spectrometer equipped with High Resolution Magic Angle Spinning (HRMAS) probe, and an indirect one fitting in vitro drug delivery data [1]. Starting from experimental data a complete overview on ESM transport properties was provided, considering the contribution of drug concentration. In particular a mathematical model that describes and rationalizes the differences between gel and water environments regarding ESM adsorption and diffusion within hydrogel pores was taken into account. The competition between these two mechanisms causes two different regimens. At low drug concentration, on one hand, adsorption prevails with a consequent diffusivity in gel lower than in water. On the other hand for high drug concentration, where all adsorption site are saturated, the diffusion in gel is similar to water solution. This study may pave the way toward the development of models able to encompass the simultaneous effect of different phenomena on diffusion for a better device design.

[1] G. Perale, F. Rossi, M. Santoro, P. Marchetti, F. Castiglione, A. Mele, E. Raffa, M. Masi. J. Biomed. Nanotechnol., 7(3), 476 (2011).

[2] M. Santoro, P. Marchetti, F. Rossi, G. Perale, F. Castiglione, A. Mele, E. Raffa, M. Masi. J. Phys. Chem. B, 2011, 115(11): 2503-2510;

DSL345
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Simulation of Post-Consumer Diapers Recycling, Sterilized By Gamma Radiation

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Despite that is not new the necessity in recycling waste, still is given little importance to proper environment dispose of diapers. Besides environmental concern, the rising difficulty in locating landfills and incinerators has encouraged public administration to look for alternatives through recycling [2]. In Brazil, several materials, that could be recycled, are still designated to dumps, generating, as well as, an environmental problem, an economical problem. After the National Policy on Solid Waste, the waste come to be considered good value, when is possible to be reused [3] [4]. Disposable diapers residues in most countries, has the final destination in landfills or incinerators and represent a large portion of waste [2]. Disposable diapers have a wide variety of natural and synthetic polymeric materials of high quality, which is desirable to reuse the same [5]. The technologies currently known to recycle diapers are not satisfactory, due to the process implementation issue, that generate large quantities of pollutants and organic waste, high energy expenditure, in addition the difficulty to promote an efficient sterilization [5]. This work aimed to research into new technologies for the recycling of post-consumer disposable diapers, using gamma radiation for sterilization and processing in conventional machines for physical transformations of polymers.

[1] A. M. Piva and H. Wiebeck, Reciclagem do Plástico, p.21, Artliber Editora Ltda., São Paulo, Brasil, 2004.
[2] J. Colón, L. Ruggieri, A. Sánchez, A. González and I. Puig, Possibilities of composting disposable diapers with municipal solid wastes, Waste Management & Research, v. 29, p.249-259, Barcelona, Spain, 2010.
[3] CEMPRE – Compromisso Empresarial Para Reciclagem, Cempre Review 2013, São Paulo, Brasil, 2013.
[4] PNRS – Política Nacional de Resíduos Sólidos, Lei n. 12.305 de 2 de Agosto de 2010, Brasil.
[5] M. Somma, G. Vaccaro, J. K. Michalek and T. Thomas, Process for Recycling Absorbent Sanitary Products, Patent Application Publication , Pub.No..: 2013/0146689 A1, p.1-3, United States, Jun/2013.

VIP052
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Current Problems with Dental Implants

Titanium and its alloys are biomaterials used for fabrication of dental and orthopedic implants as they posses several desirable physical, mechanical and chemical properties. However, efficient lifetime of existing implants is limited to 10–15 years by infection and inflammation which can result in lack of osseointegration. The prevalence of peri-implant infection in patients with dental implants has shown to range from 28–56%. Clinical cases showing the current treatment to address peri-implant infection and treatment shortcomings will be presented. Ongoing

studies using the approach of local delivery of antibiotics, will be presented. The ultimate goal of these studies are to propose the development of a novel strategy to promote the development of a self-efficient biological implant that will ultimately provide clinicians with another tool to rehabilitate patients with history chronic and acute periodontitis.

Special Session 2
FUNDAMENTAL DIFFUSION PROCESSES AND REACTIONS IN ENGINEERING MATERIALS (SS2)

DSL334
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Fractional Calculus Application in Modeling Diffusion Controlled Leaching Kinetics

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The use of fractional calculus, i.e. the use of non-integer differentiation order, is analyzed for applications in leaching operations. The diffusion controlled leaching kinetics is revised considering an anomalous diffusion due to the presence of the pore network in the substrate to be leached. Experimental published data shows that the use of fractional calculus to describe leaching kinetics is a suitable approach to describe batch leaching kinetics. This fractional calculus based diffusion is expanded to generate a simplified model for column leaching. This model is applied to experimental data of gold ore column testing. Also this is contrasted with the Fickian model in both fitting and prediction capabilities. For this application the fractional order γ of the leaching process was constrained to the interval $0 \le \gamma \le 1$. This suggest a sub-diffusive model for the gold leaching kinetics.

The fractional calculus presented a limited improvement in the fitting, but it is strongly superior to the traditional model for data prediction. In special it produces a more accurate estimated value for ultimate recovery.

DSL360
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Identification of Casting Conditions Influence on the Structure and Properties of Al-Si-X Alloy Castings by Experimental and Virtual Way

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The cast products which were not subjected to metal plastic forming are characterized by remaining in close relation with their crystallization and solidification conditions. This structure is an exploitation structure i.e. present in the casting during the entire life cycle and contains imperfections such as porosity, non-metallic inclusions and disadvantageous intermetallic phases because of the mechanical properties [1,2,3].
The initial metallurgical quality of liquid alloy depends mainly on furnace charge type, on melting conditions i.e. rate of fusion and superheating temperature, and ennobling refining method of Al-Si-X alloy (the methods of removing of non-metallic inclusions and hydrogen content) [4,5].
The metallurgical quality is assessed on the basis of at least three groups of parameters: chemical composition (spectro), the ratio of hydrogen content (Dichte index and/or the method of the first bubble (Y.Dardel method according to Sievert's law) and parameters of thermal analysis curve (DTA – Derivative Thermal Analysis).
The initial tests for high-pressure die-casting product were presented during DSL Conference in Paris in 2014 [5]. The tests concerned mainly the description of discontinuities present in microstructure like air entrapment, shrinkage and gas porosity. The comparison of casting structures made by gravity casting conditions and under HPDC conditions (High-Pressure Die-Casting) is the most effective at maintaining the same metallurgical quality during casting.
The samples made with these two methods (Gravity Die-Casting and High-Pressure Die-Casting) were subjected by mechanical properties test (static tensile test).

The fractures of ruptured specimens were subjected using fractography tests and theirs surrounding using structural tests (metallographic) [6].

The solidification models defined in relation to these conditions were served to simulate the two extremes casting processes. The results of these simulations (quality predictions) were compared with the results of the experiment. The effectiveness of applied simulation systems in terms of accuracy of thermal and structural/mechanical characteristics dynamics of casting prediction, were evaluated.

[1] Fabrizi A., Ferraro S., Timelli G., Materials Characterization, 85, 13 (2013).
[2] Vicario I. et all, 71st. World Foundry Congress, Bilbao 19-21.05.2014.
[3] Mohamed A.M.A., et all, Materials and Design, 30, 3943 (2009).
[4] D. Dispinar, et al., Materials Science and Engineering A, 527, 3719 (2010).
[5] Ignaszak Z., Hajkowski J., Defect and Diffusion Forum, 364, 80 (2015).
[6] Warmuzek M., Aluminum-Silicon Casting Alloys. Atlas of Microfractographs, (ASM International, Ohio, USA, 2004).

DSL378
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Fission Gas Generation, Diffusion and Release Fully Coupled with Fuel Deformation in a $(U_{1-y}, Pu_y)O_{2-x}$ Mixed Oxide Fast Reactor Fuel

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$(U_{1-y}, Pu_y)O_{2-x}$ fuels are widely used in fast reactor and of interest for the Generation-IV nuclear reactors, which is a promising candidate fuel not only to transmute long life minor actinides in fast breeder reactors (FBR), but also to establish a FBR cycle with high potential of non-proliferation [1]. Sodium cooled fast reactors operate with a higher linear heat rate and higher coolant temperature than Lighter Water Reactors (LWRs), and also a lower fuel smear density and lower initial oxygen to metal ratio, resulting high temperatures, high temperature gradients and a complex chemical environment [2].

During the fast reactor nuclear fuel fission reaction, new solid and gaseous species are introduced within the material. Fission gases accumulate and form pores with the increasing of fuel burnup that decrease the fuel thermal conductivity, leading to large temperature gradients. Thus nuclear fuel experiences overheating and structural changes. It is therefore expected that significant structural deformation will occur within the fuel. In order to investigate these important issues, the fission gas generation, diffusion and release, the grain growth, and the strains due to thermal expansion, irradiation-induced densification, solid fission product swelling, and gaseous fission product swelling are considered and modeled in a fully coupled way. The models are implemented into COMSOL Multiphysics to simulate the effect of the fission gas generation, diffusion and release on fuel deformation. The simulation results show that the generation, diffusion and release of fission gas bubbles plays an important role on nuclear fuel deformation.

[1] Maeda, K., et al., Radial redistribution of actinides in irradiated FR-MOX fuels. J. Nucl. Mater., 2009. 389(1): p. 78-84.
[2] Karahan, A., Modeling of thermal-mechanical and irradiation behavior of metallic and oxide fuels for sodium fast reactors, PhD thesis, Massachusetts Institute of Technology, 2009.

VIP001
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Investigation of Thermotransport of a Liquid Metal Alloy: Molecular Dynamics Study of a Ni50Al50 Melt

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We analyse the formalism of thermotransport in a binary liquid metal system with a special focus on the heat of transport that characterizes diffusion driven by a temperature gradient. We introduce the reduced heat of transport which describes that part of the interdiffusion flux that is proportional to the temperature gradient. In an isothermal system   represents the reduced heat flow (pure heat conduction) consequent upon unit interdiffusion flux. We demonstrate that   is independent of reference frame and is useful in a practical sense for a direct comparison of simulation and experimental data from different sources obtained in different reference frames. Then, we make use of equilibrium molecular dynamics simulations in conjunction with the Green-Kubo formalism to study the thermotransport properties of a model of a liquid Ni50Al50 alloy at three state points within the temperature range 1500 – 4000 K. Our results predict that in the liquid Ni50Al50 alloy in the presence of a temperature gradient Ni tends to diffuse from the cold end to the hot end whilst Al tends to diffuse from the hot end to the cold end.

DSL240
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Variation of Microhardness with Thermal Parameters and Microstructure During Transient Horizontal Directional Solidification of the Al-6.0wt.%Cu-2.5wt.%Si Alloy

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Aluminum is the second most widely used metal due to its desirable chemical, physical and mechanical properties, and it represents an important category of technological materials [1-4]. Due to its high strength-to weight ratio, besides other desirable properties, e.g., its desirable appearance, being non-toxic, non-sparking, non-magnetic, having high corrosion resistance, high electrical and thermal conductivities and ease of fabrication, aluminum and its alloys are used in a wide range of industrial applications with different aqueous solutions [1-4]. In this sense, transient directional solidification experiments were carried out with the Al-6.0wt.%Cu-2.5wt.%Si alloy in order to analyze the variation of microhardness with microstructural and thermal parameters of solidification and. The main parameters analyzed include cooling rate (TR) and primary dendrite arm spacings (l1). For this purpose, a horizontal solidification experimental apparatus was developed and specimens were solidified under transient heat flow conditions. It has been observed that for increasing values of TR the values of HV have a slight increase. On the other hand, it has been noted that HV decreases when l1 increases. Experimental laws of power and Hall-Petch type have been determined correlating HV with TR and l1, giving as results, respectively: HV = 138(TR)0.09, HV=455(l1)-0.21 and , HV=88+825(l1)-1/2

[1] C. Çadirli.. Met. Mater. Int., 19, 3, 411 (2013).

[2] D.B. Carvalho, E.C. Guimarães, A.L. Moreira, D.J. Moutinho, J.M. D. Filho, O.L. Rocha:. Mater, Research. 16,4, 874 (2013).
[3] H. Kaya; E. Çadirli; U. Böyük; N. Marasli. Appl, Surf, Sci. 255, 3071 (2008).[4] J.N. Silva, D.J. Moutinho, A.L. Moreira, I.L. Ferreira and O.L. Rocha, Mater. Chem. Phys., 130, 179 (2011).

DSL248
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Uncertainty Analysis of a Surface Catalytic Model on Silica-Based Thermal Protection Material for Hypersonic Vehicles

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Keywords: hypersonic vehicles; aerothermal heating; surface catalysis; Silica-Based TPS material; catalytic efficiency

Silica-based Material is widely employed in the thermal protection system (TPS) for hypersonic vehicles, and investigation on its catalytic characteristics is crucially important for accurate aerothermal heating prediction. Based on the eight-reaction Combined Surface Catalytic (CSC) model proposed in our previous research work, the model uncertainty caused by the variation of parameter magnitude is analyzed in this article. Results show that the characteristics of the TPS material surface, namely the concentration and radius of active sites, strongly affect magnitude of the recombination coefficient. Detailed analysis of the silica-based TPS material surface characteristics should be made to obtain the proper parameter magnitude for our CSC model. It is also shown that the magnitude of physidesorption and physidiffusion active energy has a significantly impact on the magnitude and peak position of recombination coefficient in the low temperature range. Furthermore, results show that the increase of impinging oxygen pressure will restrict the catalytic recombination, and it is in accordance with previous experimental data, thus validates our model again. These results are rather helpful for the further research on dual species (N, O) surface catalytic model.

DSL260
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Resin Transfer Molding Process Applied to Composites Manufacturing: A Numerical Simulation using PAM-RTM

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Simulation tools for Liquid Composite Moulding (LCM) processes are a key to predict and solve manufacturing issues [1,2]. Despite the fact that numerical process analyses are commonly used to predict mould filling, resin cure and exothermic temperatures, more comprehensive computational tools are still required [3]. This work aims to simulate the infiltration of a CaCO3 mixed with resin in a metallic mold filled with porous preform using the PAM-RTM software. A preform of glass fiber mat, with dimensions 320 x 150 x 3.6 mm, has been used for injection experiments conducted at room temperature, injection pressure 0.25 bar. The resin contain 10 e 40% CaCO3 content with different particles size (38 and 75 µm mesh opening). The numerical results of the flow front position were evaluated by direct comparison with experimental data. The flat flow-front profile of the rectilinear flow was reached approximately halfway the length of the mold. It was observed, that the speed of filling decreases with increasing the CaCO3 content andthe higher the amount of CaCO3 in the resin, the lower the permeability of the reinforcement is found. The reduction in permeability is due to the presence of calcium carbonate particles between the fibers, hindering the resin flow in the fibrous media. The computational fluid flow analysis with the PAM-RTM proved to be an accurate tool study the processing of composite materials.

[1] G. Palardy; P. Hubert; E. Ruiz; M. Haider and L. Lessard, Comp. Eng. 43, 824 (2012).
[2] T. Brocks; M. Y. Shiino; M. O. H. Cioffi; H. J. C. Voorwald and A. C. Filho, Mat. Res. 16, 5 (2013).
[3] I. R. Oliveira; S. A. Campos; R. Barcella and A. G. B. Lima, Defect and Diffus. Forum 353, 43 (2014)

DSL262
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Molecular Dynamics Simulation of Thermal Diffusion in Nanofluids
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Nanofluids are two-phase systems consisting of a carrier fluid and nanoparticles. The nanofluids research has both fundamental and application motivation. On the one hand the transport properties of nanofluids are not described as a rule by classical theories. On the other hand the nanofluids may be utilized in several applications, for example, engine cooling, refrigeration, thermal storage, in different biomedical technologies, and so forth. The thermal diffusion of nanoparticles is the important characteristic of the nanofluid dynamics. The experimental study of thermal diffusion of nanoparticles is pretty actively developed recently [1,2]. However such experiments are complicated enough and in them it is difficult to gain the adequate information about dependence of thermal diffusion and Soret coefficient of nanoparticles on their size, material and concentration. In this paper the thermal diffusion of nanoparticles is studied by means of the molecular dynamics method. Interaction of molecules of based fluid among themselves was modeled by potential of Lennard-Jones. Interactions of the carrier fluid molecules with a nanoparticles and nanoparticles are described by means of specially constructed potentials [3, 4], respectively. Dependences of the thermal diffusion of nanoparticles in nanofluids based on liquid argon with aluminum and zink nanoparticles are obtained. The nanoparticle size ranges from 1 to 4 nm.

[1] R. Piazza, A. Parola, J. Phys.: Condens. Matter, 20, 153102 (2008).
[2] X. Zhang, et al., Experimental Thermal and Fluid Science, 31, 593 (2007).

[3] V.Ya. Rudyak, S.L. Krasnolutskii, Proc. 21st Int. Symp. on RGD, Toulouse, G-É, 1, 263 (1999).
[4] V.Ya. Rudyak, S.L. Krasnolutskii, D.A. Ivanov, Doklady Physics, 57(1), 33 (2012)

DSL270
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Diffusion-Schrödinger Quantum Mechanics
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Keywords**:** nonlinear diffusion, quantum solution, diffusion-Schrödinger quantum mechanics, diffusion analog of the Planck constant.

A quantum solution of a nonlinear differential equation of diffusion type with a potential term has been found. Diffusion-Schrödinger quantum mechanics can find wide application in quantum biology, biological electronics, synthetic biology, nanomedicine, the quantum theory of consciousness, cosmology, and other fields of science and technology. One consequence of the macroscopic nature of diffusion-Schrödinger quantum mechanics is the possibility of generation of hard photons. The dust plasma in the Universe can generate cosmic rays with ultra-relativistic energies in a galactic magnetic field via a diffusion mechanism.

DSL292
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Ionic Conductivity in Alkali Nitrites
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Electrolytes with different type of charge carrier can find widely application in different using, e.g. sensors, electrochemical equipments, batteries and others. One of important components ensuring stable functioning of the equipment is electrolyte. Electrolyte has to be characterized by high conductivity, thermal stability, and wide electrochemical window. To many advantages characteristic for liquid electrolytes, in addition, the solid state electrolytes have good mechanical stability, wide working range of temperature range. Thus search of new system of solid electrolytes with high conductivity is an actual task of solid state chemistry. Families of alkali perchlorates and nitrates have been investigated by us earlier [1-3]. In literature data about transport properties of alkali nitrites are absent. Nevertheless, alkali nitrites MeNO2 (Me= Li+, Na+, K+, Rb+ and Cs+), except for the lithium salt, have high-temperature phases with crystal structure of the NaCl-type. High-temperature phases of nitrites are orientationally disordered, i.e. non-spherical anions are reoriented over several equivalents directions in the crystal lattice. It is very interesting to carry out an impedance study of transport properties of alkali nitrites to clarify the nature of the mechanism conductivity, type of the carrier of a charge.

In this work alkali nitrite was synthesized and its structural, thermodynamic and electrical properties were investigated. Alkali nitrite was obtained by exchange reaction from water solutions of barium nitrite and alkali sulfate. The synthesized product of reaction was several times recrystallized. The synthesized salt was characterized by X-ray powder diffraction technique using DRON-4 X-Ray Diffractometer with Cu Ka radiation. The unit cell parameter was calculated by means of Diffrac AT v3.3 program with typical accuracy of $\pm 0,005$ Å. Using thermal analysis, the temperatures of dehydration and thermal decomposition of salt were determined. Before the conductivity measurements, the salt was heated at melting temperature for 30 min, then, the dehydrated specimens were rapidly cooled, and the pellets with press-fitted silver electrodes were formed at 400 MPa. The pellets' density (in percent of theoretical density) was 0.90–0.98. The conductivity was measured using a two electrode scheme in a forevacuum (6.7 Pa) with an HP 4284A (Precision LCR meter) in a frequency range 20 Hz $< v < 1$ MHz.

Conductivity of $MeNO_2$ was investigated by a complex impedance technique. The values of conductivity are well reproduced in the heating–cooling cycles and are stable under the long-term exposure in a vacuum under the isothermal conditions. In the series of nitrite of alkaline metals Li^+-Cs^+, the conductivity varies not monotonically with increasing radius of cation. The minimum conductivity is observed for potassium perchlorate; however, with further increase in the radius of cation in the series, the conductivity tends to increase. The most interesting results were obtained for caesium nitrite. Pure $CsNO_2$ has rather low ionic conductivity, near $5*10^{-8}$ S/cm at 25^oC, and good conductivity, near 10^{-3} S/cm at 350^oC. Such a behavior of conductivity may be explained by the presence of segments with own and impurity conductivity. Activation energy of high temperature segment point to ionic character of conductivity. For clarification of the nature of the charge carrier additional experiments on Hebba-Wagner's method on tablets with carbon electrodes, on Tubandt's Method and doping by isovalent impurities (e.g. Ba^{2+}) were carried out. Results of experiments are discussed in the report.

[1]. A.S. Ulihin, N.F. Uvarov, B.-E. Mellander, Solid State Ionics, 179, p. 228 (2008).
[2]. N.F. Uvarov, A.A. Iskakova, A.S. Ulihin, N.N. Medvedev, Solid state Ionics, Vol. 188, 1, p.78, (2011).
[3] A.S.Ulihin, N.F.Uvarov, Yu.G.Mateyshina, L.I.Brezhneva, A.A.Matvienko, Solid State Ionics, 177, p. 2787 (2006).

DSL297
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Effects of Vanadium on the Continuous Cooling Transformation of 0.7 %C Steel for Railway Wheels

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One of the ways to reduce the cost of cargo transport in railways is increasing the amount of cargo carried in each wagon. For this, the wheel must have a higher hardness to withstand wear, however, without loss of ductility and toughness. To achieve the required levels of hardness, railway wheels with microalloyed steels are being developed. These steels contains small amounts (less than 0.5% by mass) of niobium, vanadium or titanium. To understand the effect of these element on the microstructure and related mechanical properties of the steels the CCT diagrams are required. In this work, CCT diagrams for 0.7 C, 0.4 Mn and 0.9 Si steel without (steel 7C) and with 0.12 V addition (steel 7V) were constructed. Microstructures produced in the range between 0.5 and 100 ºC/s were analyzed with optical microscopy, XRD, TEM and SEM. Vanadium refined the austenitic grain (12 and 6 mm for 7C and 7V, respectively), what can be explain by the presence of fine (10 nm in diameter) V_4C_3 precipitates, which restricts the austenitic grain growth. In addition, vanadium, in solid solution, reduced the pearlite interlamelar

spacing (0.13 and 0.11 mm for 7C and 7V, respectively) by depressing the initial temperature pearlite formation (644 and 639 °C for 7C and 7V, respectively). He increased the ferrite volume fraction from 1 to 3 % at cooling rate of 1 ºC/s, due the fact that vanadium is a ferrite stabilizer. Vanadium addition did not affect the initial temperature for martensite formation, but increased the hardenability with martensite formation at slower cooling rates (10 and 5 ºC/s for 7C and 7V, respectively). For higher cooling rates (20 to 100 ºC/s), the austenite transformation to martensite at room temperature was incomplete and all steels presented martensite and retained austenite, which volumetric fraction was near the same for both steels varying from 20 to 40 %.

[1] AAR MSRP, 2011, "Manual of Standards and Recommended Practices Section G" – Wheel and Axles, M-107/M-208.
[2] A. A. Barani et alii, Materials Science and Engineering: A, v. 463, p. 138-146, (2007).

DSL300
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Phonons Scattering by Substitutional Impurities in a Quasi-3D Nanostructure

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In the present work we investigate the influence of crystalline reticular defect on the elastic waves propagating through a nanostructure modelled by two infinite monatomic plans. The study is confined to the elastic scattering in the harmonic approximation framework. The problem is tackled from a semi-classical point of view, using scattering boundary conditions and applying the matching method formalism. This theoretical approach, based on the Landauer-Büttiker principle, permits to determine the dynamics of the perfect waveguide and allows one to carry out the phonons localized induced states, the displacements of the perturbed region atoms, the transmission and reflection coefficients of the perturbed system. This matching method combined with the Green's functions theory allows one also to determine the densities of states (DOS) of all irreducible atoms in the perturbed region. Numerical results show that the presence of defect in the structure modifies particularly its mechanical and vibrational properties by the creation of new localized states by bulk and surface phonons scattering. Its influence results in a general decrease of the transmission probability amplitude accentuated by Fano-like resonances and/or Fabry-Pérot oscillations. The transmission spectra, obtained by scattering experiments, could then be regarded as fingerprints of the specific defect structure. The results could be also useful for the design of phonon devices and provide a basis for the understanding of conductance spectroscopy experiments in mesoscopic systems.

[1] B. Kramer, Quantum Coherence in Mesoscopic Systems, (plenum, New York, 1991).
[2] R. Landauer, J. Phys. Condens. Matter, 1, 8099 (1989).
[3] M. Büttiker, Phys. Rev. Lett., 57, 1761 (1986).
[4] M. S. Rabia, J. Phys.: Condens. Matter 20, 465318 (2008); Physica E 42, 307-1318 (2010).

DSL302
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Structural Evolution of Cold Compacted Al-Co Alloy System

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A set of Al-Co binary alloys (with respectively in weight percent 10%, 20%, 30%, 40%, 50% and 60% Co)   have been studied by X-ray diffraction at the as compacted state.

The structural evolution according to cobalt addition shows special features as the apparition of fcc cobalt and hcp cobalt beside aluminium in some cobalt compositions of the Al-Co mixtures using only cold compaction without sintering at high temperature. Figure 1

Cobalt is not a common alloying element in aluminium because its solubility is very low [1].

According to the pressure–temperature phase diagram, Co is known to exist in two allotropic forms: a low-temperature hcp phase and a high-temperature fcc phase [2-3]. At room temperature, Co is stable in the hcp form but it transforms to the fcc form when it is heated to above the transition temperature 695K.

Powder aluminium and cobalt (99.999 %) were used in the proportions defined according to the required compositions. The total mass of the samples to be elaborated was between 8 g

and 10 g. Cold compaction of mixed powder (Al-Co) under an uniaxial load of 10 MPa has been achieved to obtain a dense product (60%).
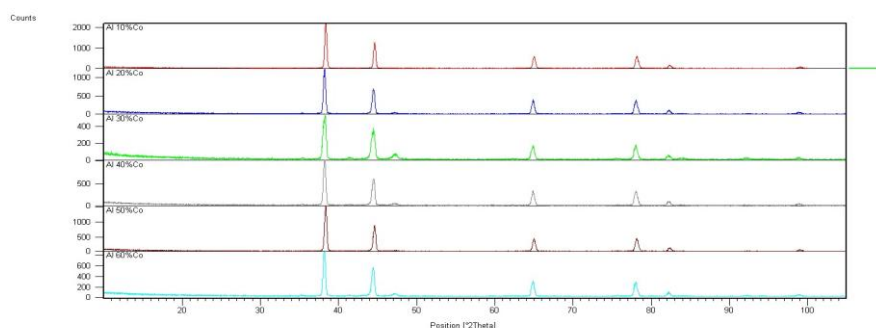
Figure 1.X-Ray diffraction patterns of compacted Al-Co alloys.

References

[1] J. Sort, J. Nogue, S. Surin, M. D. Baro: Philosophical Magazine, Vol. 83, 2003, No. 4, p. 439-455, DOI: 10.1080/0141861021000047159

[2] S. Sun, C.B. Murray: Journal of applied Physics, Vol. 85, 1999, No. 8, p.4325-4331, DOI: 10.1063/1.370357

[3] A. Fekrache, M. Y. Debili, H. Boularas, D. Lamrous, N. Sassane, Acta Metallurgica Slovaca, Vol. 20, 2014, No. 1, p. 50-59 50

DSL314

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Transformation-Induced Plasticity in Super Duplex Stainless Steel UNS S32760

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Due to their unique combination of properties Super Duplex Stainless Steels (SDSSs) are materials of choice in many industries. Their applications and markets are growing continuously and without any doubt there is a great potential for further volume increase.

In recent years, intensive researches have been performed on lean SDSSs improving mechanical properties exploiting the lack of nickel to generate metastable γ-austenite, resulting in transformation-induced plasticity (TRIP) effect.

In the present work, UNS S32760 SDSS have been studied coupling its microstructural features, especially secondary austenitic precipitates, and tensile properties, after different thermal treatments. First, the investigated specimens have been undergone to a solution thermal treatment at 1300° C and, then, to an annealing treatment at 1080° C with different holding times. The results of microstructural investigations and mechanical testing highlight the occurrence of TRIP processes. This feature has been related to the Magee effect, concerning the secondary austenitic precipitates nucleated via martensitic-shear transformation. [2]

[1] J.Y. Choi, J.H. Ji, S.W. Hwang and K.-T. Park, Mater. Sci. Eng. A, 535, 32 (2012)
[2] L. Taleb and S. Petit, Int. J. Plasticity, 22, 110 (2006)

DSL325
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Diffusion of Chromium in Nickel Base Alloys: Application to Stress Corrosion Cracking

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Intergranular Stress Corrosion Cracking (IGSCC) of nickel base alloys is one of the major degradation phenomena in the primary circuit of Pressurized Water Reactors (PWR). IGSCC occurs by the combination of stress, material and environment and leads to a brittle fracture of a ductile material. Understanding this mechanism is a key issue concerning the prolongation of reactor lifetime. Recently, a model of IGSCC based on selective oxidation of chromium at the crack tip has been presented in the literature [1]. At the crack tip, the author observed chromium oxide associated with a chromium depleted layer of about 20 nm in the grain and 200 nm along the grain boundary. This depleted zone would be formed in about 6000 seconds [1]. He concluded that one of the key steps of the SCC mechanism could be chromium diffusion in Alloy 600 (Ni-15Cr-10Fe). There is very little literature data concerning the diffusion of chromium in nickel base alloys in the temperature range between 300 and 600°C. The aim of this work is to determine if under certain test conditions, chromium diffusion in Alloy 600 could explain the formation of the chromium depleted zone. Chromium diffusion tests in pure nickel and Alloy 600 single-crystals are performed on non-deformed, pre-deformed samples and on specimen loaded during a creep test. Diffusion profiles are measured by Secondary Ion Mass Spectrometry (SIMS). The surface imaging mode in SIMS is also presented and results are compared with those obtained by depth profile mode.

[1] M. Sennour, P. Laghoutaris, C. Guerre, R. Molins, Journal of Nuclear Materials, 393 (2009) 254-266

DSL330
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Analysis of Self-diffusion in Ionic Liquids

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Study of self-diffusion in ionic liquids is an important property as the diffusion of both cation as well as of anion is to be measured as a function of both the temperature and the pressure. At present, the experimental data for self-diffusion are available as a function of temperature in pure imidazolium-based ionic liquids like [C1C2Im][CH3SO4],[C1C4Im][CH3SO4], [C1C2Im][CF3SO3] and [C1C4Im][CF3SO3].

The aim of the present paper is to analyze the behavior of self-diffusion of these ionic liquids as a function of temperature in the temperature range 298 K to 343 K. For this purpose, a model is suggested which is capable of representing the experimental data very well as a function of temperature. As an illustration, the computed results of self-diffusion, based on the model, in ionic liquid [C1C2Im][CH3SO4]*** is compared with the experimental data in the table given below. A very good agreement is found between the experimental results and the computed data in case of each liquid which gives the confidence in the model used.

Table: Comparison between experimental and calculated values of self- diffusion coefficient (10-11m2/s) in ionic liquid [C1C2Im][CH3SO4]***

DSL331

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Brazing Vacuum Ceramic Tubes – A Diffusion Profile in the Joint

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The Sirius Project is an initiative of the Brazilian Synchrotron Light Laboratory - LNLS (CNPEM - MCTI), for the design, construction and operation of a new synchrotron radiation source 3rd generation, with high brightness and energy of the electrons of 3.0 GeV. Among many other components, will be built 80 ceramic cameras embedded in specials magnets, whose function is to act to correct the orbit of the electron beam in the storage ring. The ceramic chamber is crucial for this application because this material is transparent to the magnetic field generated in the electro magnet and thus acts directly on the electron beam. The difficulty of these constructive components lies in the fact that, the ceramic components must be attached to metal components will join vacuum chambers that make up the ring, and then must present excellent mechanical and vacuum tight. The process of chemical bonding between the ceramic and metal components is performed by brazing in high vacuum. After brazing, is deposited a film of copper with 7 micrometers thickness. The objective of this paper is to describe the process of film deposition and brazing of copper and the excellent results obtained in the production, mechanical characterization, microstructural and tightness.

1. http://lnls.cnpem.br/sirius/ Sirius: the New Brazilian Synchrotron Radiation Source, access 09/01/2014.

2. 3. BAGNATO, O. R., GARCIA JR, O. R. AND FRANCISCO, F R. The Influence of Superficial Roughness in the Mechanical Resistance of Alumina / kovar Joints. 6th Brazilian MRS Meeting October 28 th – November 1st. SBPMat 2007.

DSL344
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A Dilatometric Study of the Non Isothermal Structural Evolution of a Cold Rolled Al 6060 Alloy

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The Al-Mg-Si alloys are widely used in the form of sheets and plates for various structural applications. Sheets or plates for structural applications may be produced by the conventional rolling. To control the microstructure of the final product, to obtain specific properties and performance, it is necessity to monitor closely and/or predict microstructural transformations during the industrial processing. To the authors' knowledge, while isothermal aging of deformed Al–Mg–Si alloys has been extensively studied, relatively few reports document the non isothermal aging of deformed Al–Mg–Si alloys. The knowledge of anisothermal aging of deformed Al–Mg–Si alloys is very essential to understand the thermal stability of its microstructures as well as to control the microstructure of the final product during industrial processing which often involve non-isothermal aging. Therefore, the present work has been focused to understand the microstructural evolution during the continuous heating of a deformed Al6060 alloy. The microstructural evolution has been investigated using dilatometry, Differential Scanning Calorimetry, X-ray Diffraction and microhardness measurement. The deformed sample shows a new dilatometric behavior. Based on the different results, the occurrence of the new dilatometric anomalies has been explained by the competition between recovery and precipitations reactions at low temperatures and the dissolution and recrystallization reaction at higher.

DSL361
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Diffusive Process of Ceramic Material Produced with Lapidary Waste and Chitosan Biopolymer

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Keywords: Ceramic Material, Lapidary powder, Chitosan, Fick's Law.

The Valley Mucuri, in Minas Gerais, Brazil, is seated in one of the largest gemological provinces in the world, given its size and diversity of gemstones ranging from diamond to amethyst and citrine. The stoning segment is one of its most important economic activities and, in the region there is approximately 300 micro areas of stoning and marketing. The material to be cut generates waste minerals such as crushed stone, and this in turn damages the environment causing air pollution and impact on the landscape. The adoption of alternative use of this residue will add value to this material for industrial use. In this case, the ceramic industry stands for the ability to co-process waste and one of the items especially those with physical and chemical properties to suit the peculiarities of the

production process and can enable benefits to industry and process. This study aimed to obtain ceramic ceramics using powder semi-precious stones from stonecutters Mucuri Valley with addition of biopolymer chitosan. Therefore, specimens of samples Were prepared for sintering temperatures in the 850 ° C and 1100 ° C Were Subjected to mineralogical characterization tests, chemistry and physics. The properties evaluated were aiming to present to discuss results of a preliminary study of diffusion in ceramic materials in this material were: Chemistry Fluorescence X-Ray, Water absorption (%), Scanning Electron Microscopy, SEM and process the Forward using Fick's Law.

DSL362
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Multiphase Ni–Cr–Al Diffusion: A Comparison of Bi-Velocity Phase Field Simulations with Experimental Data

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The bi-velocity (Darken) phase-field method is applied to simulate the interdiffusion in the two-phase zone of Ni-Cr-Al system. The extended bi-velocity method allows calculating the local material velocity and entropy production in the system that undergoes the overall volume change. For the first time we consider different partial molar volumes of the components and show quantitative evaluation of phase distribution. The results of calculations are compared with experimental data at 1473 K. The diffusion multiples were prepared by hot isostatic pressing (HIP), at 200 bar and 1473 K. HIP technique allows obtain good junction between terminal alloys and prevents oxidation. The simulation results are in good agreement with the experimental data.
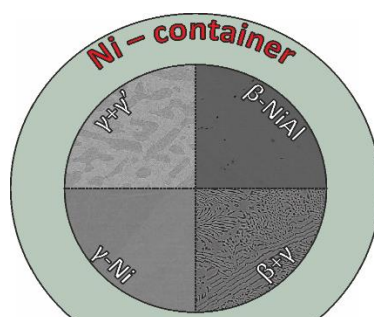

Fig. 1 Multiphase diffusion multiple – positions of the terminal alloys.

DSL373
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Enhanced Mathematical Modeling of DOP Plasticizer Migration from PVC into Liquid (methanol)
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Polyvinyl chloride, commonly abbreviated PVC is a rather hard and rigid material. In order to extend its use it requires additives during the manufacturing process which are referred to as plasticizers, among them the Dioctyl Phthalate (DOP) . This latter has a tendency to escape from the PVC matrix specially when in contact with liquids. In order to analyse this phenomenon we use the classical equations of mass diffusion (Fick's second law) . However this method leads to results which are not always in good agreement with experimental ones , especially when the concentration of plasticisers is high. This situation requires the elaboration of an enhanced mathematical model that can deal with this particular type of forced diffusion characterized by the contact of a liquid and particular boundary conditions. The validation of the proposed model was obtained by comparing the theoretical results obtained with the model and those obtained by experiments.

Key words: DOP, forced diffusion, mathematical model.

DSL385
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Comparative Analysis of Atomic Transport Properties of 5D Liquid Transition Metals using Different Reference Systems
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In the present study, we have calculated atomic transport properties like self diffusion coefficient (D) and viscosity coefficient (η) of 5d transition liquid metals. We have been used one component plasma (OCP) reference system to describe structural information alongwith our newly constructed parameter free model potential. To see the effect of different correction functions on atomic transport properties, we have used different local field correction functions like Hartree (H), Sarkar et al (S) and Taylor (T). From the present results we have concluded that our newly constructed model potential successfully calculated atomic transport properties of 5d transition metals in liquid phase.

DSL392
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Effect of Temperature and Aging Factor on Wettability Alteration by Cationic Surfactant (DTAB)
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Applications of surfactants for wettability alteration in oil-wet reservoir rocks has been suggested for many years now by researchers. The importance of surfactant flooding is featured since carbonate reservoirs (oil-wet reservoirs) form almost 50% of the total reserves in the world. In this experimental study, the effects of temperature and aging time has been studies on wettability alteration in understudied limestone rocks using cationic surfactant, Dodecyl Trimethyl Ammonium Bromide (DTAB). The results indicate a noticeable impact of temperature and aging time on contact angel reduction. A correlation between contact angle as a function of surfactant concentration and aging time has been offered for the case study.

[1] Seethepalli A., Adibhatla B., and Mohanty K.K., SPE 89423,(2004).
[2] Standnes, D.C. and Austad, T., "C&S: P&A, 216, 243-259. (2003)

DSL397
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Crystallization Kinetics in Cu50Zr43Al7 Bulk Metallic Glass

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Crystallization kinetics of a Cu50Zr43Al7 bulk metallic glass was investigated through differential scanning calorimetry (DSC) in isothermal mode using Johnson–Mehl–Avrami model. Samples were prepared by copper-mold casting method. Amorphousness of the as-cast samples was confirmed by XRD. Each DSC curve of the BMG exhibited an incubation period followed by an exothermic peak corresponding to the crystallization of the amorphous phase indicating that the devitrification of Cu50Zr43Al7 BMG has followed a one-stage process. The activation energy for crystallization was about 471 kJ/mol obtained by the Arrhenius equation. The Avrami exponent was determined to be 2.2 implying that the crystallization is governed by three-dimentional interface-controlled growth. At the end, fragility index was also calculated and discussed.

Keywords: Bulk metallic glasses, Crystallization kinetics, Avrami exponent, differential scanning calorimetry

DSL413
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Investigating Kirkendall Effect in Thin Films by Experiments and Simulations

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It is well-known, that Kirkendall shift can occure in binary systems. We investigated Kirkendall effect in thin films on the nanometer scale by experiments and computer simulations. Since on this length scale the characteristic distances between the vacancy sinks and sources can be comparable to the dimensions of the sample, the usual vacancy annihilation processes, leading to the classical Kirkendall shift, cannot operate. Experiments were

performed on Fe-Sb system, computer simulations were performed in the framework of the new conceptual model of Erdélyi & Schmitz. (Erdélyi & Schmitz, 2012)

References

Erdélyi, Z., & Schmitz, G. (2012). Reactive diffusion and stress in spherical geometry. Acta Materialia, (60) 1807-1817.

DSL246
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Age Hardening and Accompanying Transformations of the Alag and Alcumg Supersaturated Solid Solutions

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In this paper, the development of the transition metastable phases and the hardening accompanying their evolution are studied for Al-20%(wt)Ag and Al-3%(wt)Cu-1%(wt)Mg.These supersaturated solid solutions (α^*) are quenched and decompose following the precipitation sequence

α^*_{AlAg} ⟶ GP zones γ' ⟶ γ ⟶

α^*_{AlCuMg} ⟶ GPB zones S'' ⟶ S' ⟶ S ⟶
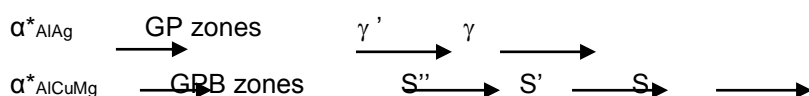
where the clusters GP (Guinier-Preston) and GPB (Guinier-Preston-Bagaryatsky) zones form by a process of a negative diffusion. γ', S'', S' are the metastable phases.

They attain their equilibrium state (γ and S) after several phases transformations. During this evolution to the equilibrium phase it appears an important hardening which then decreases. The metastable phases are characterized on the isotherms hardness and their temperature range is determined on the isochronal hardness.

DSL343
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Liquid - Solid Transformation in Magnetic Induction Fused Al-Zn Alloys

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Four binary Al-Zn alloys containing nominally 4.38, 15, 21.5 and 29.2 at % Zn were synthesized by fusion under high frequency induction (HF). The structural characterization was carried out by X-ray diffraction (XRD), optical microscopy, scanning electron microscopy (SEM), energy dispersive X-ray (EDX).

Results of these investigations show that the microstructure of all alloys consists of α-Al dendrites and eutectic in interdendritic regions. Al-15 at.% Zn alloy presents a columnar-equiaxed transition (CET) from hydrodynamic flow of liquid in contact with columnar dendrites. The structure of Al-21.5 at.% Zn and Al-29.2 at. %Zn alloys is characterised by cellular dendritic grains. The presence of impurities elements (Fe, Si) allows an intermetallic phase of (Al,Fe,Si)3,6Zn type and different morphologies of precipitates.

Key words: Al-Zn, microstructure, HF fusion, phase transformations, impurities

DSL099
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Modeling Phases Formed during Boriding for Estimation Depth Boron Through the Growing in Substrate by Lattice Boltzmann Method

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The boriding process is a thermochimical threatement, used to produced hard and wear resistant coatings on iron alloys in witch the atom of boron diffuse in the substrat, usualy metalic. [1]
In the industry we are interested in the nature of the layer well as the thickness of the boride layer. The Fe 2 B phase is desirable [2], hence the interest in our study.
The most approach , used in simulation of on the diffusion of boron in iron substrate, don't take in order the collision between the boron atom and those of substrate [3,4,5,6] whatever considering substrate or interstitial diffusion [7], this work is a try to applicat the Boltzmann theory about collision [8] between atoms during the diffusion of boron in the interface FeB / Fe2B. [9]
The collision of atoms causes a disorder which Boltzmann quantified as the state function which is expressed by entropy [10]. The study of the diffusion process we are interested in this work is based on the thermodynamic approach and in particular the entropy state function at the boron atom diffusion in a metal substrate and simulation the variation of the concentration of boron of the Fe 2 B phase as a function of the thickness of the layer form diboride. We took our calculations we consider a function f which expresses the probability of the presence of a certain amount of atoms in a given time and at a treatment temperature set
We compared the results of digital processing that reached through a computer code written in Visual Fortran, with published literature [11] and we obtained a good match.

References :
[1] I. Campos-Silva, J. Martínez-Trinidad, M.A. Doñu-Ruíz, G. Rodríguez-Castro, E. Hernández-Sánchez, O. Bravo-Bárcenas , Surface & Coatings Technology, 206, 1809 , (2011) .
[2] O. Allaoui , N. Bouaouadja , G. Saindernan, Surface & Coatings Technology, 201, 3475, (2006).
[3] A. Schneider, G. Inden, Acta Materialia 53, 519–531, (2005).
[4] O. Culha, M. Toparli, T. Aksoy, Advances in Engineering Software, 40, 1140–1147, (2009).
[5] I. Campos, G. Ramırez, U. Figueroa, J. Martınez, O. Morales, Applied Surface Science, 253, 3469–3475, (2007).
[6] M. Keddama, M. Ortiz-Domınguez, I. Campos-Silva, J. Martınez-Trinidad, Applied Surface Science, 256, 3128–3132, (2010).
[7] Z. Nait Abdellah , M. Keddam, A. Elias, ACTA PHYSICA POLONICA A , 122, 588-592, (2012).
[8] Dieter Wolf-Gladrow, Journal of Statistical Physics, Vol. 79, Nos. 5/6, 1023-1032, (1995).

[9] C.S. Bresolin, A.A.M. Oliveira, Computer Physics Communications 183, 2542–2549, (2012.)

[10] Héctor A. Martínez-Berumen, Gabriela C. López-Torres, Laura Romo-Rojas , Procedia Computer Science, 28, 389 – 390, (2014) .

[11] M. Keddam, Applied Surface Science, 236, 451–455, (2004).

DSL202

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Study of the diffusion processes in the Fe-Al system induced by the Spark Plasma Sintering / Field Assisted Sintering Technology

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Spark Plasma Sintering (SPS) / Field Assisted Sintering Technology (FAST) is an advanced sintering technique utilizing pulsed electrical direct current (DC) at low voltages and uniaxial pressure. The application of electrical field effects leads to enhanced reactivity and sinterability compared to conventional sintering methods making the FAST attractive for conducting solid state synthesis [1]. The investigation of diffusion processes in the system Al-Fe under influence of pulsed DC provides the basis for controlled reactive solid state FAST to produce tailored compact Al-Fe materials.

In this study, the growth of intermetallic phases evolving due to the interfacial reactions in the diffusion couple Al-Fe-Al was analysed. Samples were produced at temperatures between 450°C and 600°C for 30 min to 120 min. The rising temperatures are inseparably related to increasing RMS DC densities between 64 A/cm2 and 133 A/cm2. The scanning electron microscopy (SEM) including electron back-scattered diffraction (EBSD) and WDX was employed to reveal microstructural features in the diffusion zone, identify the sequence of intermetallic phases and conclude their growth behavior.

The product layers contained the intermetallic phases Al13Fe4 (C2/m) and Al5Fe2 (Cmcm). The Al13Fe4 phase appeared thin and uncontinuous. The Al5Fe2 phase was the main constituent phase in the reaction layer. It consisted of columnar grains with a pronounced crystallographic [001] orientation with respect to the growth direction. The Al5Fe2 layer grew according to the parabolic growth law. The imposition of the pulsed DC strongly enhanced the growth kinetics independent on the current direction. A rate constant k of $1.4 \cdot 10^{-11}$ m2/s at 600°C with 133 A/cm2 was found. In comparison, Jindal et al. [2] determined a rate constant k of $1.5 \cdot 10^{-13}$ m2/s at 600°C without an applied DC.

[1] Z. A. Munir, U. Anselmi-Tamburini and M. Ohyanagi, J. Mater. Sci. 41, 763 (2006).

[2] V. Jindal, V. C. Srivastava, A. Das and R. N. Ghosh, Mater. Lett. 60, 1758 (2006).

DSL213

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Concentration-Dependent Self-Diffusion Coefficients in Amorphous Si1-xGex Solid Solutions; an Interdiffusion Study

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Amorphous semiconductors, such as Si, Ge or their solid solutions Si1-xGex are applied in many state-of-the-art technologies such as thin-film photovoltaic devices and thin-film transistors. Knowledge of diffusion in such amorphous semiconductors is of vital importance for processing and application of these devices. However, owing to the challenging experimental investigation, current knowledge about diffusion in amorphous semiconductors is very limited. In this study, interdiffusion in amorphous Si/ Si0.52Ge0.48 multilayers, prepared by thermal evaporation, has been investigated at 440 °C - 460 °C by Auger electron spectroscopy (AES) sputter-depth profiling and by applying the Mixing Roughness Information depth (MRI) model[1,2] to account for sputter induced alternations of the measured intensity-depth profiles. This analysis allows to reveal diffusion lengths in the nanometre range and, in contrast to X-ray and neutron diffraction studies, to account directly for the concentration dependence of the diffusion coefficients in the amorphous Si1-xGex system (for x< 0.48). From the established concentration-depth profiles, concentration-dependent self-diffusion coefficients could be deduced. The deduced concentration dependence and activation enthalpy of self-diffusion coefficients in amorphous Si1-xGex are explained by the covalent bonding nature of the atoms in the amorphous phase. The observed considerably larger self-diffusion coefficients in the amorphous phase, as compared to those in the crystalline phase, suggest that the free volume inherent in the amorphous phase facilitates diffusion, and a cooperative diffusion mechanism may operate in the amorphous phase.

[1] S. Hofmann, Surf. Interface Anal., 27, 825 (1999)
[2] M. A. Noah, D. Flötotto, Z. M. Wang and E. J. Mittemeijer, Surf. Interface Anal., 46, 1057 (2014)

DSL238
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Diffusion Processes Modeling with the Bi-Flux Approach
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Consider a set p of particles spreading along a given path. At a given time a subset of p, say p2=(1−β)p , due to some reason, is forced to decrease the spreading speed. It is possible to think that the flux rate variation is due to the reduction of the particle´s energy expended to produce the diffusion effect. This phenomenon could be triggered by some change in the internal metabolism of the particles composing the subset p2 or the modification of the particle´s casing geometry or physicochemical properties. We may think of living cells, or other living organisms which are subject to changes which may interfere in the speed of the scattering process. If we are dealing with population dynamics, for instance, it is possible to consider a population subset subjected to some disease that reduces the capacity to move at the same pace as the healthy group. In any case, there will be two groups of the set p, p1= βp and p2=(1−β)p diffusing with two different flux rates. Note that the supporting medium is the same for both groups meaning that the diffusion coefficient D is constant for both cases. The flux rate corresponding to the population p2 is clearly different from the flux rate corresponding to p1 but this is due to the intrinsic modification of the constituents involved in the process. That is to say that we cannot model the diffusion process with two classical diffusion equations with different diffusion coefficients: pt=Dipxx i=1,2. The introduction of reactive terms, we think, would be artificial for this case. We propose a new approach to this situation where the diffusing elements play an active role in the flux rate. So, let us assume that the primary group consisting of the fraction β of the total population spreads according the classical Fick´s rule, say f1~px. The secondary group

consists of the complementary fraction (1−β). It is shown that a consistent derivation of the governing equation [1] [2], preserving the mass conservation principle, leads to the conclusion that the secondary flux rate should be proportional to the third derivative of the density function, f2~(β pxx)x. Note that the secondary flux exists if and only if the primary flux exists, that is f2≠0 if and only if β≠0. The governing equation is now a fourth order PDE of the form pt= βDpxx − β(1−β)Rpxxxx. A new parameter R appears in the equation which depends on the characteristics of the population p2.

Another application of the bi-flux approach, although in different context, is modeling capital flux in a given economy. For this case the primary flux is related to the amount of capital inflow and the secondary flux corresponds to capital outflow. That is the primary and secondary fluxes have opposite directions. By summing up both amounts it is possible to determine the tendency of the economy that could be growth, decay or stagnation. It is suggested that the different tendencies are partially determined by the parameter R, controlling the secondary flux, that could be associated to the tax rates. For this model it is also convenient to add capital sources and sinks induced by the internal players in the economic system. Therefore the diffusion approach as presented here may also be introduced to deal with capital flow in a simple economic system, a small industry for instance, instead of the discrete model traditionally used to analyze this class of problems [3] [4].

[1] L. Bevilacqua , A. C. N. R. Galeão , F. P. Costa, An. Acad. Bras. Cienc., 83, 1443 (2011)
[2] L. Bevilacqua, A. C. N. R. Galeão, J. G. Simas, A. P. Rio Doce, J Braz. Soc. Mech. Sci. Eng., 35, 431 (2013)
[3] J.B. Barro, N.G. Mankiw, X. Sala-i-Martin, Center Discussion Paper no.655, (Economic Growth Center, Yale University, 1992).
[4] P.O. Gourinchas, J. Olivier, Working Paper Series, WP 09 - 12, (Peterson Institute for International Economics, 2009).

DSL275
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Effects of Quantization on the Thermal Activation of Formation and Migration of Mono-Vacancies in BCC Iron

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In a recent calculation [J. Nucl. Mater. 455(2014)31], entropies and enthalpies of vacancy formation and diffusion in BCC iron are calculated as a function of temperature. Magnon contributions in this calculation are found to be particularly substantial near the ferro/para-magnetic transition, resulting in strong temperature dependence and singular behavior can be seen in this temperature regime, reflecting magnon softening effects. The phase-space trajectories used in this calculation are obtained using spin-lattice dynamics simulations performed using a heat bath based on the classical fluctuation-dissipation theorem.

However, in this classical treatment of thermal activation of atomic processes in crystalline materials, energy quantization is neglected and all vibration modes can be excited independent of temperature. This may lead to a generic over-estimation of the amount of thermal energy available to drive the activation and hence its rate of the process. In this presentation, we perform our calculation using a Langevin heat bath based on a fluctuation dissipation relation formulated according to the Bose-Einstein statistical description of the energy distribution of thermal excitations in terms of phonons and magnons. The results are compared with our former calculation, in which quantization effects are neglected. Significant differences are found except for temperatures near the Curie temperature. The results are discussed.

DSL283
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Enhanced Diffusion and Direct Transport on Magnetic Garnet Films

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In this talk, I will review several recent discoveries related to the controlled diffusion and transport of paramagnetic colloidal particles above magnetic garnet films [1]. The garnet films are thin uniaxial ferromagnetic films in which ferromagnetic domains can be organized into symmetric patterns consisting of stripes or bubbles and generate strong local magnetic field gradients. Application of an external homogeneous magnetic field on a larger scale compared to the spatial periodicity of the magnetic pattern in the film modulates the potential generated at its surface and induces the controlled motion of colloidal particles placed above the film. Several novel dynamical regimes are observed and reported, from localized trajectories to direct particle transport, depending on the geometry of the underlying magnetic pattern and on the parameters, which control the external driving field, such as frequency, strength and direction. [2,3]

[1] P. Tierno, F. Sagués, T. H. Johansen, T. M Fischer, Phys. Chem. Chem. Phys., 11 9615 (2009).
[2] P. Tierno, P. Reimann, T. H. Johansen, F. Sagués, Phys. Rev. Lett., 105, 230602 (2010).
[38] P. Tierno, Phys. Rev. Lett. 109, 198304 (2012).

DSL311
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Oxidation Behavior of a Novel Si-Containing Cr-Mn-C-N Austenitic Stainless Steel in Dry Air Atmosphere at 1000⁰c

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Keywords: austenitic stainless steel, high temperature oxidation, silica, reactive element.

The isothermal oxidation behavior of a novel Si-containing Cr-Mn-C-N austenitic resistant steel in dry air atmosphere at 1000⁰C was investigated by weighting method, X-ray diffraction, scanning electron microscope and electron probe micro-analyzer. The results showed that the oxidation kinetics of the steel approximately followed a cubic law. A continuous protective oxide scale formed on the surface of the steel. This oxide scale consisted of outer layer of spinel ($MnFe_2O_4$), middle layer of M_2O_3 ((Mn, $Cr)_2O_3$ and Cr_2O_3) and inner layer of silica (SiO_2). Based on the experimental observation, the oxidation mechanism and the synergistic effect of Cr, Si and Ce on the oxidation resistance were discussed.

DSL321
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Dissolution in Layered Ni (Solid) – Al (Liquid) thin Films
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The dissolution of one phase A into another phase B seems to be a simple problem. It is transient phenomenon that occurs until the concentration of A in B reaches the solubility limit. If A is in solid state and B is liquid, the dissolution must take place through the interface. In the case of a nanometric multilayer, the system is made with interfaces that are just separated by a few nanometers. Despite the large number of interfaces, the dissolution could be hindered by the microscopic processes, which became predominant at nanoscale. The kinetics associated with the phase transformation Asol → Aliq at the interface Asol/Bliq can be controlled by the interface itself since the A atoms have to cross an atomic barrier. In other situations, the kinetics is limited by the diffusion of A atoms into B liquid. The effective rate of dissolution depends on the microscopic mechanism.

In this work, we have studied the dissolution process of Ni into liquid Al in a layered Ni-Al-Ni system by means of molecular dynamics simulations, using an embedded-atom method type potential. Concomitantly, we have developed a diffusion model of the dissolution process. The model based on classical Fick's laws allows estimating the solubility limit of Ni in a liquid alloy Ni+Al for different temperatures. The observed dependence can be associated to the liquidus line of the phase diagram and can be extrapolated to predict the melting temperature of pure Ni. Also, the diffusion coefficients of Ni in the liquid alloy were obtained in the temperature range from 1100 K to 1600 K and correlate quite well with experimental data. An Arrhenius fit gives an estimation of the activation energy of $Q = 43.7$ kJ/mol and of the prefactor $D_0 = 6.57 \cdot 10^{-7} m^2/s$. The present study demonstrates the predominant role played by diffusion in the dissolution process at nanoscale in layered systems.

DSL329
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Internal Stress Assisted and Concentration Dependent Diffusion of Nitrogen in Alloys during Nitriding at Moderate Temperature
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The nitriding of alloys (such as austenitic stainless steels (ASSs) and CoCr alloys) at moderate temperatures (below formation of nitrides) generates a precipitate free hardened surface layer which consists mainly of a metastable phase, known as supersaturated or expanded austenite. Expanded austenite phase is characterized by the expansion of the alloy lattice and an anomalous plateau type nitrogen diffusion profiles which are very different from standard complementary-error-function-like diffusion (erfc-shape Fick's diffusion) profiles. In this work the interstitial nitrogen diffusion in CoCr alloy and ASS is investigated on the basis of internal stress assisted diffusion model. Proposed model assumes that the stress field, associated with the distorted alloy lattice due to incorporation of nitrogen, influences the diffusive flux of nitrogen. There are two driving forces for nitrogen diffusion: concentration gradient and internal stress gradient. The last one can be understood as barodiffusion in solids. By considering of experimental depth profiles, it was found that nitrogen diffusion coefficient in ASS and CoCr alloys varies with nitrogen concentration according to Einstein-Smoluchowski relation $D(C_N) = f(1/C_N)$. With the increase

of nitrogen content in austenite, the occupancy of the interstitials in lattice increases. As a result, the probability that activated nitrogen atom can jump to an unoccupied site is reduced and, as a result, the diffusion coefficient decreases. The expansion of the alloy lattice because of incorporation of nitrogen leads to swelling process. It is shown, that experimental depth profiles registered for different nitriding times can be fitted by one the same Onsager coefficient only in the case if swelling process is assumed. The swelling is confirmed and measured in many experiments and calculated values correspond with experimentally measured ones. The proposed diffusion model, which includes the internal stresses, concentration dependant diffusion and swelling, was successfully applied for theoretical analysis of experimentally obtained nitrogen diffusion profiles for different types of ASS and medical grade CoCr alloys at different experimental conditions. The kinetics of nitriding processes is analyzed by proposed model.

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Ab Initio Modeling of Copper Impurity Diffusion in Tin

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TiN is an important material used as a diffusion barrier to prevent copper from contacting silicon in microelectronic devices. There is however little known about the elementary processes at the atomistic level underlying the excellent performance of TiN. The scarce experimental data presented in literature has a significant spread due to following reasons: 1) TiN has a high melting point; 2) Samples used for diffusion studies differ in stoichiometry and crystallinity. To the best of our knowledge, on the theoretical side there are only work by Tsetseris and co-workers [1], where a number of mechanisms of Cu diffusion in TiN have been considered and the corresponding activation energies have been calculated using density functional theory (DFT). Though the study reported in Ref. [1] advance our understanding of impurity diffusion in titanium nitride significantly, questions remain worth of further investigation. One of such questions is the effect of off-stoichiometry, which has been treated so far in qualitative manner.

In this work we make an attempt to quantitatively estimate the effect of the off-stoichiometry of TiN using the first principles approach based on DFT. To this end we calculate concentrations of the intrinsic point defects in titanium nitride as a function of composition via the grand-canonical thermodynamic formalism based on the dilute solution model [2]. We study the site preference of Cu impurity atoms on the TiN sub-lattices by calculating the corresponding defect formation energies, again taking into account the effect of off-stoichiometry. Finally, we calculate the stoichiometry-dependent diffusion coefficients for three diffusion mechanisms: interstitial and vacancy-driven diffusion on the Ti- and N-sublattices.

[1] L. Tsetseris, S. Logothetidis, S.T. Pantelides, Appl. Phys. Lett., 94, 161903 (2009)
[2] C. Woodward, M. Asta, G. Kresse, J. Hafner, Phys. Rev. B, 63, 094103 (2001)

DSL339
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Tracer Diffusion Studies in Equiatomic FCC High Entropy Alloys

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High entropy alloys (HEAs) are multicomponent alloys having constituent elements in equiatomic or near-equiatomic ratios. These alloys possess unique attributes like multi-prinicpal elements, sluggish diffusion kinetics, enhanced thermal stability and superior wear and oxidation resistance. In particular, HEAs with FCC structure have been explored for high temperature applications, for which creep behavior and in turn the diffusion kinetics of these alloys must be understood. In this work, first results on diffusion kinetics in 4, 5 and 6 component HEAs viz. CoCrFeNi, CoCrFeMnNi and CoCrFeMnNiV will be reported. Tracer diffusion coefficients for Ni, Fe, Cr and Co will be determined using appropriate radioactive isotopes.

The alloys were prepared by arc melting the constituent elements in equiatomic proportion, followed by homogenization at 1200°C for 50 h. X-ray diffraction results reveal that CoCrFeNi and CoCrFeMnNi have single phase FCC structure, while CoCrFeMnNiV comprises of FCC and tetragonal phases. A single phase structure, uniform composition and a grain size in excess of 250 microns is revealed in Electron Back-Scattered Diffraction (EBSD) results of CoCrFeNi and CoCrFeMnNi alloys. Elemental x-ray maps of CoCrFeMnNiV substantiate its decomposition into a Ni- and Mn-rich phase (located predominantly at grain boundaries) and a V- and Cr-rich phase.

DSL365
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Phase Formation and Diffusion Kinetics Analysis of Al-Based Multilayer thin Films by Atom Probe Tomography

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Phase formation behavior for polycrystalline multilayer (ML) thin films with negative heat of mixing is similar in common binary Al-based systems such as Ni/Al, Ru/Al, Ti/Al, Nb/Al, Co/Al, and Ag/Al [1]. The early-phase formation strongly influences the phase evolution, which is far from equilibrium conditions. The kinetics in this case is mainly governed by four factors: the film deposition conditions, the film internal stresses, the fast-diffusion paths, and the period thicknesses, respectively [2]. Although the extensive numerical and experimental work that has been carried out over the past almost three decades to explain the role of such factors on phase formation in MLs, the resulting interdiffusion as a function of these factors remains unclear.

An in-depth experimental analysis at the atomistic level on Al-based MLs using atom probe tomography (APT) is presented here. The results highlight the effect of two deposition parameters (deposition rate and Argon pressure) and ML period thickness on grain boundary (GB) diffusion and interfacial mixing. APT offers a uniquely high spatial resolution (~0.1 nm) to precisely analyze interfaces in thin films. However, this precision cannot be reached for all materials due to measurement artifacts originating from non-uniform field evaporation along interfaces [3]. The work here therefore mostly focuses on a ML system which maintains the high resolution capability of the technique but also represents the common phase formation behavior in Al-based MLs. Preferential nucleation sites, concentration gradients and GB diffusion types are reported. Differential scanning calorimetry, X-ray diffraction, transmission electron backscatter diffraction and scanning transmission electron microscopy techniques were also used to characterize the films.

[1] G. Lucadamo, K. Barmak, S. Hyun, C. Cabral, C. Lavoie, Mater. Lett., 39, 268-273 (1999).
[2] N. Zotov, K. Woll., F. Mücklich, Intermetallics, 18, 1507-1516 (2010).

[3] F. Vurpillot, D. Larson, A. Cerezo, Surf. Interface Anal., 36, 552-558 (2004).

DSL374
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On The Consistency of Onsager's Reciprocal Relations in Various Reference Frames;
A Critical Test of the Bi-Velocity (Darken) Method by Entropy Calculations

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An appropriate choice of reference frame for diffusion in multicomponent systems is a prerequisite to define fluxes and velocities of the components. Despite a long-standing discussion of this subject its unified treatment in view of Onsager's irreversible thermodynamic formalism is still lacking. On account of this, we present a critical discussion on the consistency of Nernst-Planck and Onsager approaches relative to various reference frames: (i) material reference frame, (ii) laboratory reference frame and (iii) R-th component reference frame. It is shown that for the fluxes and forces given by linear combinations, $\sum_{i=1}^{R} a_i J_i = 0$, $\sum_{i=1}^{R} b_i X_i = 0$ and $J = MX$, one can define new sets of forces $\tilde{X}$ and fluxes, $\tilde{J} = L\tilde{X}$, that are interrelated with symmetric matrix of phenomenological coefficients: $L = \left(L_{ij} \right)_{i,j=1\ldots R-1}$, $L_{ij} = L_{ji}$ and this matrix is explicitly defined.

The problem is considered dichotomously, i.e. (a) for equal molar volumes of the components, $\sum_i c_i = const$ and (b) for various molar volumes of the components, assuming Vegard's rule, $\sum_i c_i \Omega_i = 1$. In critical test of the results the entropy production calculated from the general formula for the local entropy production rate $\dot{\sigma} = \sum_i X_i J_i$ has been compared with the entropy change calculated from a difference of mixing entropy in the final and initial states: $\Delta S = S_{final} - S_{initial}$. The calculations have been made for the interdiffusion in the ternary Fe-Ni-Co diffusional couple. A perfect agreement has been achieved.

Table I. The analysing scheme.

Reference frame	Approaches		
	a) **Nernst-Planck** $\sum_i c_i = const$	b) **Nernst-Planck** $\sum_i c_i \Omega_i = 1$	**Onsager** $\sum_i c_i = const$
(i) Material reference frame R diffusion fluxes	Symmetric $\left(M_{ij} \right)_{i,j=1,2,\ldots,R}$ matrix of phenomenological coefficients: $M_{ij} = M_{ji} = 0$		Symmetric $\left(M_{ij} \right)_{i,j=1,2,\ldots,R}$ matrix of phenomenological coefficients: $M_{ij} = M_{ji}$
(ii) Laboratory reference frame Darken interdiffusion fluxes			
(iii) R-th component reference frame The problem reduced to $R-1$ components	Symmetric $\left(L_{ij} \right)_{i,j=1,2,\ldots,R-1}$ matrix of phenomenological coefficients		

DSL389
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Origin of Size Dependent Concurrence of Grain Growth and Phase Transition: A Deep Insight from Thermodynamics and Kinetics

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Concurrence of grain growth and phase transition are ubiquitous in condensed matter physics; however, the thermodynamics and kinetics involved which is critical to understand the concurrence remains scarcely studied. Here, we performed a systematic study of probing the interaction between phase transition and grain growth by adjusting the grain size when phase transition is triggered. Our study indicates as the grain size decreases the measured enthalpy change decreases, and both transition kinetics are more strongly influenced. Furthermore, we give a full description of the thermodynamic driving force and kinetic activation energy of every individual elemental process, suggesting a reverse correlation exists for both two solid reactions. Our findings clearly provide a comprehensive picture on the size-dependent concurring kinetics of grain growth and phase transition, and show a method to tailor the interaction in between, which could be easily extent to other material system.

VIP027
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Diffusion and Ionic Conduction in some Oxide Glasses

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Diffusion and ionic conduction are closely related phenomena. Diffusion is conveniently studied by tracer techniques, which monitor the long-range transport of ions tagged by their radioactivity. The dc conductivity of an ion-conducting solid is measured by impedance spectroscopy and reflects the long-range transport of ionic charge. In contrast to ionic conduction, tracer diffusion is element-specific.

This contribution reviews tracer experiments which comprise measurements of ^{22}Na and ^{86}Rb diffusion in single and mixed alkali borate glasses and of ^{22}Na and ^{40}Ca diffusion in soda-lime silicate glasses as function of temperature, pressure and composition [1-6]. Diffusivities and dc conductivities are Arrhenius activated and are compared via the Nernst-Einstein relation and yield Haven ratios. Viscosity diffusion coefficients are deduced from viscosity data for soda-lime silicate glass via the Stokes-Einstein relation. Viscosity diffusion is considerably slower than diffusion of the network modifiers Na and Ca indicating that the motion of the network formers and network modifiers are decoupled. The ionic conductivity in soda-lime glasses is dominated by Na ions. The contribution of Ca ions is negligible

The influence of hydrostatic pressure on diffusion and ionic conduction was studied for Na-Rb borate glasses. The activation volume of ionic conduction is relatively small on the Na-rich side, it is larger on the Rb-rich side. The

activation volumes in the single alkali glasses correlate with the ionic volumes of Na or Rb ions. The activation volume increases to a shallow maximum in the mixed alkali range. This observation is a fingerprint of the so-called mixed-alkali effect in addition to the minimum of the ionic conductivity and the maximum of the activation enthalpy of ionic conduction. The activation volumes of tracer diffusion are significantly larger than those of ionic conduction in both, single and mixed-alkali glasses. The tracer diffusivities have a stronger pressure dependence than the dc conductivity. The observations indicate that the mechanism of the ionic jump process varies with pressure and temperature, which we attribute to a varying degree of collectivity of the ionic jump process.

1. S. Voss, F. Berkemeier, A. W. Imre, H. Mehrer, Z. Phys. Chem. 218, 1353-1374 (2004)
2. S: Voss, A. W. Imre, H. Mehrer, Phys. Chem. Chem. Phys. 6, 3669-3675 (2004)
3. A. W. Imre, S. Voss, H. Mehrer, Defect and Diffusion Forum 237-240, 370-383 (2005)
4. F. Berkemeier, S. Voss, A. W. Imre, H. Mehrer, J. Non-Cryst. Sol. 351, 3816-3825 (2005)
5. A. W. Imre, S. Voss, F. Berke-meier, H. Mehrer, I. Konidakis, M. D. Ingram, Solid State Ionics 177, 963-969 (2006)
6. A. W. Imre, H. Staesche, S. Voss, M.D. Ingram, K. Funke, H. MehrerJ. Phys. Chem. B 111, 5301 -5307 (2007)

VIP033
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The Reduction Processes of the Titaniumcontaining Iron Ores Treatment

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Questions of metallurgical processing of titaniumcontaining ores are considered. Tests of ores and concentrates of the Ural deposit [1] - low-titanous and high-titanous are studied. Reducibility, durability, temperatures of a softening and melting of iron ore pellets are in vitro studied. Are carried out phase and a X-ray the structural analysis. Calculations by means of mathematical models of pyrometallurgical processes [2, 3] are executed. Possibility of processing of these ores according to schemes is shown: «blast furnace melting - converter melting» and «metallization - electromelting».

[1] A.N. Dmitriev, G.Yu. Vitkina, R.V. Petukhov et. al. The Characteristic of Ores and Concentrates of the Open Society "EVRAZ KGOK" / Advanced Materials Research (Volumes 834 - 836). 2014. P. 364-369.
[2] Chentsov A.V., Chesnokov Yu.A., Shavrin S.V. Logic-statistic balance model of blast furnace smelting process. 164 p. Ekaterinburg: Ural Branch of Russian Academy of Sciences. 2003.
[3] Dmitriev A.N. Mathematical modeling of blast furnace process. 163 p. Ekaterinburg: Ural Branch of Russian Academy of Sciences. 2011.

VIP034
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Diffusion in LiNbO3 at Low Temperatures

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Lithium niobate (LiNbO3) is a technologically important oxide with an extraordinary combination of ferroelectric, piezoelectric, acoustic, optical, and ion-conducting properties. For many applications, Li self-diffusion close to room temperature is of high importance. Examples are thermally induced ionic re-arrangements for an optimization of optical properties, tailoring of ion-conductivity by structural/defect disorder, and the formation, stability and dissociation of defect clusters and their influence on ferroelectric properties. We carried out systematic experiments on Li diffusion in LiNbO3 single crystals as well as in amorphous films below 500 °C. For analysis we used 6LiNbO3/7LiNbO3 isotope heterostructures in combination with Secondary Ion Mass Spectrometry [1,2] and Neutron Reflectometry [3,4].

The diffusivities in congruent LiNbO3 single crystals follow the Arrhenius law with an activation enthalpy of 1.33 eV and are identical within error limits to diffusivities calculated from impedance measurements. This indicates that Li is the dominating species governing conductivity down to 200 °C. The diffusivities of near stoichiometric single crystals are lower by a factor of about ten, while the activation enthalpy is identical. This supports the existence of a (NbLi4Ÿ + 4 vLi/) defect structure to explain off-stoichiometry. The Li diffusivities in amorphous lithium niobate are about ten orders of magnitude higher than that of the crystalline counterparts, while the activation enthalpy is reduced to 0.70 eV. This is attributed to Li migration in a more loosely packed amorphous structure.

[1] J. Rahn et al., Phys. Chem. Chem. Phys. 14 (2012) 2427.
[2] J. Rahn et al. Z. Phys. Chem. 226 (2012) 439.
[3] E. Hüger et al. Phys. Rev. B 85 (2012) 214102.
[4] E. Hüger et al. Phys. Chem. Chem. Phys. 16 (2014) 8670.

VIP036

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Thermodynamic Model For Mg-Si Couples Formation Kinetics In Al-Mg-Si Alloys

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Based on the trapping concept [1,2], a thermodynamic model describing the Gibbs energy of the system accounting for Mg-Si couple formation in an Al-Mg-Si matrix is developed. The equilibrium concentration of dimers is obtained by minimizing the Gibbs energy of the system for fixed temperature, chemical composition and the trapping energy describing the energy gain due to Mg-Si couple formation relatively to monomers of Mg and Si atoms. The evolution equations describing the kinetics of dimer formation are derived by means of the Thermodynamic Extremal Principle [3]. The kinetics is controlled by the superposition of two processes: i) Mg atoms are considered as immobile traps and Si atoms can diffuse and fall into the traps, ii) Si atoms are considered as immobile traps and Mg atoms can diffuse and fall into the traps. The studies based on this process concept can significantly contribute to a better understanding of the early stages in nucleation of complex precipitates. The predictions of our model for equilibrium states are compared to similar approaches in open literature, such as the model of Howard and Lidiard [3], which uses a different approach to the treatment of the configurational entropy and provides different results.

[1] J. Svoboda and F.D. Fischer, Acta mater., 60, 1211 (2012).
[2] J. Svoboda, Y.V. Shan, E. Kozeschnik and F.D. Fischer, Modell. Simul. Mater. Sci. Eng., 21, 065012 (2013).
[3] F.D. Fischer, J. Svoboda and H. Petryk, Acta mater., 67, 1, (2014).
[4] R.E. Howard and A.B. Lidiard, Rep. Prog. Phys., 27, 161 (1964).

VIP038
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Oxygen Ion Conducting Materials for Energy Conversion and Data Storage
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Interest in materials exhibiting oxygen ion conduction has increased during the last years owing to their great importance for energy and environmental applications, such as solid oxide fuel cells for converting chemical to electrical energy, solid oxide electrolyzer cells for high-temperature electrolysis of water, oxygen permeation membranes for separating oxygen from air, reversible oxygen storage–release materials to store oxygen, and catalysts to develop efficient and ecofriendly chemical processes.

Ceria-based oxides are regarded as key oxide materials for energy applications due to the fact that rare earth-doped ceria is a pure oxygen ion conductor while undoped ceria is a mixed oxygen ion–electron conductor. Using density-functional theory (DFT) we have investigated defect formation energies and entropies and oxygen migration energies as well, both in undoped and in rare earth-doped ceria. The macroscopic oxygen ion conductivity was then investigated by means of Kinetic Monte Carlo (KMC) simulations. We show that all interactions between the defects, namely vacancy-dopant attraction, dopant-dopant repulsion and vacancy-vacancy repulsion as well contribute to the so-called conductivity maximum of the ionic conductivity. We also demonstrate that ordering of the cations is one source of long-term degradation of the oxygen ion conductivity.

In contrast to the above, high-temperature applications oxygen ion conductivity at room temperature can be utilized for resistive switching of oxides. We will discuss recent examples for amorphous, highly-nonstoichiometric oxides.

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Chemical ordering Phenomena in Nanostructured FePt: Monte Carlo Simulations
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Monte Carlo (MC) simulation studies of free-surface-induced selective destabilization of L10 superstructure variants in nanolayered FePt [1,2] were extended upon nanowires and nanoparticles. The system was modeled with nn and nnn interatomic pair interactions deduced from "ab-initio" results for Fe-Pt [1]. [100]-oriented nanowires and nanocubes of the system limited by (100)-type free surfaces were simulated by respectively imposing or not

imposing 1D [100] periodic boundary conditions upon the generated L10 cubic supercells built of 256000 lattice sites. The generated samples initially perfectly ordered in the c-variant L10 superstructure ((001)-oriented monoatomic planes) and containing 1 vacancy were relaxed at temperatures between 1100 and 1500 K with the Glauber MC algorithm implemented with vacancy mechanism for atomic migration. The heterogeneous nucleation of a- and b-L10 variant domains reported previously for FePt nanolayers [1] was now induced by all the (100)-type surfaces limiting the nanowires and nanocubes. While the initial c-variant L10 superstructure of nanowires transformed totally to the L10 a-variant with Fe and Pt monoatomic planes perpendicular to the wire axis and to both (010) and (001) surfaces, in the case of nanocubes the competinion between the a- and b-variant L10 domains nucleating at the (100), (010) and (001) surfaces resulted in suppression of their growth. As a consequence, most of the cube volume remained untransformed and showed the c-variant L10 chemical long-range order (LRO) with a degree lowered by homogeneously creating antisite defects. The results quantified by the calculated a- and b-L10 domain penetration depth and the LRO and SRO degree in particular cases are important for the development of magnetic storage media technologies requiring stable L10 superstructure variants determining easy magnetization directions.

[1] M. Kozłowski, R. Kozubski, Ch. Goyhenex, V. Pierron-Bohnes, M. Rennhofer, S. Malinov, Intermetallics 17, 907-913, (2009).
[2] M. Rennhofer, M. Kozlowski, B. Laenens, B. Sepiol, R. Kozubski, D. Smeets, A. Vantomme, Intermetallics, 18, 2069-2076, (2010).

VIP043
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Self- and Interdiffusion in Liquid Alloys
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In recent years, the study of self-diffusion in liquid metals and their alloys made a significant step forward by using Quasielastic Neutron Scattering (QENS) in combination with classical container-based [1] sample processing as well as levitation techniques [2]. Newly developed in-situ X-ray [3] and neutron [4] radiography based techniques for studying chemical diffusion enabled to identify disturbing influences adding to mass transport. Both QENS and radiography allow for overcoming these additional contributions to mass transport and, hence, they enable accurate measurements of transport coefficients to a high precision. With this high precision data it is possible to discuss in more detail the relation between self- and interdiffusion in liquid alloys. Here, recent data on the Zr-Ni, Al-Ni, Al-Cu, and Al-Ag binary as well as the Al-Ag-Cu ternary eutectic will be presented. Zr-Ni is a densly-packed system with a pronounced chemical short range order. Mass transport properties for this system will be discussed in detail and compared with mode-coupling theory calculations based on measured partial structure factors [5]. For Al-Ni, which is also a system with a pronounced chemical short-range order, cross correlations significantly contribute to chemical diffusion even at very low Ni concentrations [6]. For the binary systems Al-Cu a detailed discussion on self- and interdiffusion and their relation to viscous flow is presented. For the ternary eutectic E1 of Al-Cu-Ag the full matrix of diffusion coefficients and their relation to the binary constituents is discussed [7].

[1] F. Kargl, H. Weis, T. Unruh, and A. Meyer J. Phys. Conf. Series 340, (2012) 012077.
[2] A. Meyer, S. Stüber, D. Holland-Moritz, O. Heinen, and T. Unruh, Phys. Rev. B 77 (2008) 092201.
[3] F. Kargl, E. Sondermann, H. Weis, and A. Meyer, High Temp.-High Press. 42, (2013) 3.
[4] F. Kargl, M. Engelhardt, F. Yang, H. Weis, P. Schmakat, B. Schillinger, A. Griesche, and A. Meyer, J. Phys. Condens. Matter 23, (2011) 254201.

[5] P. Kuhn, J. Horbach, F. Kargl, A. Meyer, and Th. Voigtmann, Phys. Rev. B 90, (2014) 024309; P. Heintzmann, F. Yang, and A. Meyer (unpublished).
[6] E. Sondermann, F. Kargl, and A. Meyer (unpublished).
[7] M. Engelhardt, PhD Thesis RWTH Aachen (2014); M. Engelhardt, D. Heuskin, B. Ignatzi, F. Kargl, and A. Meyer (unpublished).

VIP050
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Bombardment Induced Ion Transport through Ion Conducting Glasses: Analysis of Conductivity and Diffusion Profiles

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Recently, we have reported a new experimental approach for determining the ionic conductivity of a broad range of materials ranging from ion conducting glasses to pol-ymer films and even polyelectrolyte membranes [1,2,3,4]. The approach is based on bombarding the surface of the sample with an alkali ion beam. The soft landing of ions on the sample surface causes a well defined surface potential. The backside of the sample is connected to a grounded metal electrode. The potential gradient and the concentration gradient arising from this adsorption induce ion transport through the sample which is detected as a current on the backside electrode. The technique is termed bombardment induced ion transport (BIIT).

If the bombarding ion and the conductor ion are identical measuring the ion current at the backside electrode as a function of the kinetic energy of the bombarding ions pro-vides access to highly accurate ionic conductivities.

If the bombarding ion is not present in the sample prior to bombardment BIIT induces an electro-diffusion profile in the sample, which we are able to analyze by means of ToF-SIMS (time of flight secondary ion mass spectrometry). The entire diffusion pro-files can be quantitatively described based on a Nernst-Planck-Poisson theory both in the case of a glass [5,6] and of a polymer film [7]. This analysis provides additional information on the space and concentration dependence of diffusion coefficients.

 In this talk I will demonstrate the current capabilities and limitations of the technique. We cannot only analyze material properties but also severely manipulate material properties in particular in the interface region. Possible applications include e.g. the surface hardening of glass. In the case of glasses the experiment is capable of ad-dressing the mixed alkali effect [8]. In the case of polymer films and polyelectrolyte membranes we can investigate the conductivity of ultra-thin samples. The thinnest sample investigated so far was a PEM bilayer with thickness of ca. 4nm. Current inter-est is aimed at the formation of interphases between the electrolyte material and a metal electrode.

[1] M. Schäfer and K.-M. Weitzel, PCCP, 2011, 13, 20112-20122
[2] P.V. Menezes, J. Martin, M. Schäfer, H. Staesche, B. Roling, K.-M. Weitzel, PCCP, 2011, 13, 20123-20128
[3] S. Schulze, J. Zakel, M. Schäfer, A. Greiner, K.-M. Weitzel, PCCP 2013, 15, 1481-1487
[4] The Weitzel and Parak groups, Macromolecular Rapid Communications, 2013, 34, 1820–1826
[5] L. Rossrucker, P.V. Menezes, J. Zakel, M. Schäfer, B. Roling, K.-M. Weitzel, Z. Phys. Chem. 2012, 226, 341-353
[6] J. Zakel, P.V. Menezes, M. Schäfer, K.-M. Weitzel, Solid State Ionics 2013, 242, 20-25
[7] S. Schulze, J. Zakel, M. Schäfer, K.-M. Weitzel, IEEE-TDEI 2012, 19, 1167-1174
[8] D. Budina, J. Zakel, J. Martin, P.V. Menezes, M. Schäfer, K.-M. Weitzel, Z. Phys. Chem. 2014, 228, 609–627

VIP054

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Tracer and Interdiffusion in NiAl/NiAlTi Couples

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NiAl-based alloys represent not only crucial components of technologically important materials but also an attractive playground for testing of fundamental concepts in solid state diffusion, since numerous datasets were accumulated so far. Recently, an approach was formulated which allows determination of the composition dependence of tracer diffusion coefficients in binary and multi-component alloys using a single diffusion couple [1].

In the present study, such an approach is tested against a number of couples of the systems Ni49.2Al46.1Ti4.7/64Ni/NiAl and Ni49.2Al46.1Ti4.7/44Ti/NiAl. The end-composition of binary NiAl was varied between the stoichiometric Ni50Al50 and Ni-rich Ni55Al45 alloys. Both quasi-binary as well as ternary diffusion couples were investigated recording chemical diffusion profiles of all three components and the concentration distributions of 63Ni and 44Ti radioisotopes on identical samples. The results are discussed with respect to applicability of the approach [1].

[1] Belova IV, Kulkarni NS, Sohn YH, Murch GE, Phil Mag 94 (2014) 3560.

DSL219
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Development of Microstructure and Properties of Mg-Y-(Nd)-Zn Alloys during Heat and Mechanical Treatment

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This work is focused on development of microstructure and properties of Mg-Y-Zn and Mg-Y-Nd-Zn alloys during heat and mechanical treatment. In the as cast state both alloys exhibit almost equiaxed grains with little larger size in Mg-Y-Zn alloy with grain boundaries decorated by different structures - long period ordered structure (LPSO) was detected in Mg-Y- Zn alloy and eutectic structure of Mg3Nd type in alloy with Nd addition. High density of stacking faults is evident in both alloys.

Both alloys were repeatedly isochronally heat treated from room temperature up to 440 °C. Resistivity and microhardness measurement was performed after each heating step. Stacking faults persist both annealings in both alloys and microhardness development shows no remarkable differences. LPSO in Mg-Y-Zn alloy disappear after the first annealing and was again detected after repeated annealing up to 340 °C. No LPSO development was observed in Mg-Y-Nd-Zn alloy. After the whole treatment no grain growth appeared.

Differential scanning calorimetry measurement was performed for both repeatedly heated alloys up to 540 °C. There are three exothermic peaks in DSC curves of Mg-Y-Zn alloys that can be ascribed to embedding solute atoms in stacking faults, LPSO development and transformation and coarsening of grain boundary particles. DSC curves of Mg-Y-Nd-Zn alloy where no LPSO was observed exhibit two exothermic peaks that probably correspond to solute atoms embedding in stacking faults and development of thin basal plates.

Measurement of microhardness after sequential deformation of both alloys in the as cast state was performed. The alloys were cold rolled in steps of 0.9 % thickness reduction up to cracks formation. Strengthening of both alloys is very similar but formation of cracks in the alloy with Nd addition begins after lower reduction (about 14 %) compared to Mg-Y-Zn alloy (about 18 %).

DSL378
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Plutonium and Oxygen Diffusion in a (U1-y, Puy)O2-x Mixed Oxide Fast Reactor Fuel

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It is well know that in uranium-plutonium mixed oxide (MOX) fuels, plutonium and oxygen migrate against the temperature gradient during irradiation in fast reactors [1-3], which operates at high fuel temperatures, together with a steep temperature gradient. The diffusion of the fuel constituents under the temperature gradient driving force becomes very active. Plutonium and oxygen tend to redistribute through the fuel pellet. This behavior affects the fuel temperature distribution and power distribution.

Plutonium and oxygen diffusion with the high temperature gradient is one of the important fuel performance concerns in fast reactor (U1-y, Puy)O2-x fuel during irradiation, and will affect nuclear fuel materials properties, power distribution and overall performance of the fuel pin. This study focuses on the plutonium, oxygen and heat diffusion within (U1-y, Puy)O2-x fast reactor fuel pellets. In this study, the (U1-y, Puy)O2-x fuel properties are modeled for thermal conductivity, specific heat, plutonium diffusion and oxygen diffusion. Three dimensional burnup dependent oxygen diffusion, plutonium diffusion and heat diffusion models are fully-coupled to account for the effects on each other. The models are implemented into COMSOL Multiphysics to perform this analysis. The fuel radial temperature was found to be very sensitive to O/M ratio distribution at small fractions of plutonium content. For larger fractions of plutonium content, the effects of O/M ratio and plutonium distributions are equally important.

[1] Lassmann, K., The OXIRED Model for Redistribution of Oxygen in Nonstoichiometric Uranium Plutonium Oxides, J. Nucl. Mater., 1987. 150(1): p. 10-16.
[2] Clement, C.F. and M.W. Finnis, Plutonium Redistribution in Mixed Oxide (U, Pu)O2 Nuclear Fuel Elements, J. Nucl. Mater., 1978. 75(1): p. 193-200.
[3] Ishii, T. and T. Asaga, An investigation of the Pu migration phenomena during irradiation in fast reactor, J. Nucl. Mater., 2001. 294(1-2): p. 13-17.

VIP001
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Self- and interdiffusion phenomena in triple-defect B2-ordering binary system: Monte Carlo simulation

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A binary A-B system mimicking Ni-Al was modeled with nn and nnn interatomic pair interactions yielding B2 chemical ordering and the tendency for triple-defect-type disordering. Temperature-dependent equilibrium atomic configuration in the system including equilibrium vacancy concentration and distribution was determined by means of Semi Grand Canonical Monte Carlo (SGCMC) simulations. Following the technique developed previously for the same system modeled with nn interatomic pair interactions, self diffusion of A and B atoms in equilibrium atomic configuration of the system completed with saddle-point energies for atomic jumps to nn and nnn vacancies was simulated with a Kinetic Monte Carlo (KMC) algorithm involving both types of jumps. The evaluated diffusivities of the system components yielded thermodynamic activation energies of the process, which were then analysed in terms of the applied model and the effect of B2 long-range order.

In the second stage of the study the interdiffusion dynamics in A1+xB1-x/A1-xB1+x diffusion couple was KMC simulated. Two variants of simulations were run: Within the first variant the couple showing initially the SGCMC-determined equilibrium atomic configuration and the vacancy concentration was simulated by means of canonical KMC. In the second variant, the KMC simulations were accompanied by parallel equilibration of local vacancy concentration according to SGCMC results corresponding to local chemical composition generated in the couple by the interdiffusion process. The intrinsic diffusion coefficients of A and B atoms following from both KMC simulation variants were determined within the Boltzmann-Matano formalism. Finally all the simulation results were compared and analysed in terms of the Onsager-Manning theoretical considerations.

VIP075
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From Reaction-Controlled Uptake to Uphill Diffusion:
Unprecedented Insight into Mass Transfer by Micro-Imaging
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As an omnipresent phenomenon in nature, diffusion is among the rate-determining processes in many technological processes. This is in particular true for mass separation and catalytic conversion in nanoporous materials [1]. The talk illustrates the possibilities of exploring mass transfer in such "host" materials by microscopic measurement, i.e. by the direct observation of intrinsic diffusion phenomena. Microscopic diffusion measurements include the observation of the propagation pattern of guest molecules by the pulsed field gradient technique (PFG) of NMR, notably by recording the probability density of molecular displacements as a function of the observation time (referred to as the mean propagator [2]). Such type of measurement, which recently has been shown to be applicable to also exchangeable cations [3], provides direct access to intracrystalline diffusivities and to both their impediment (by additional transport resistances due to intrinsic and/or surface barriers [4]) and enhancement (by mesoporosity [5,6]).

Though providing, at least in principle, the potentials of directly recording intracrystalline guest diffusion under also non-equilibrium conditions, following the example given in ref. [7] most of the applications of MR imaging to nanoporous materials did, so far, deal with the measurement of long-range diffusion in zeolite assemblages. Thus, our potentials for diffusion studies with nanoporous materials have been notably reinforced by the recent advent of the techniques of microimaging [8], notably by interference microscopy (IFM) and IR microscopy (IRM). In this way, transient guest profiles, well known as theoretical patterns from the Crank and Carslaw-Jaeger text-books, became accessible by immediate experimental observation. Examples of insight so far inaccessible (if not even unthinkable) include the quantification of transport resistances on the surface of the individual crystallites [9], the exploration of the interrelation between tracer (or self-) diffusion and transport (or chemical or collective) diffusion of guest molecules [10] and the observation of guest-induced variations in the host lattice [8]. As particular highlights in the exploitation of these novel options, microimaging was most recently successfully applied to the

first direct measurement of the effectiveness factor of catalytic reactions [11] and to the observation of uphill diffusion, i.e. of diffusive fluxes into the direction of increasing concentration.

[1] J. Kärger, D.M. Ruthven, and D.N. Theodorou, Diffusion in Nanoporous Materials, Wiley - VCH, Weinheim, 2012.
[2] J. Kärger, and W. Heink, J. Magn. Reson. 51 (1983) 1–7.
[3] S. Beckert, F. Stallmach, H. Toufar, D. Freude, J. Kärger, and J. Haase, J. Phys. Chem. C 117 (2013) 24866–24872.
[4] J. Kärger, ChemPhysChem 16 (2015) 24–51.
[5] J. Kärger, and R. Valiullin, Chem. Soc. Rev. 42 (2013) 4172–4197.
[6] D. Mehlhorn, R. Valiullin, J. Kärger, K. Cho, and R. Ryoo, Chem. Phys. Chem. 13 (2012) 1495–1499.
[7] W. Heink, J. Kärger, and H. Pfeifer, Chem. Engi. Sci. 33 (1978) 1019–1023.
[8] J. Kärger, T. Binder, C. Chmelik, F. Hibbe, H. Krautscheid, R. Krishna, and J. Weitkamp, Nature Materials 13 (2014) 333–343.
[9] L. Heinke, and J. Kärger, Phys. Rev. Lett. 106 (2011) 074501.
[10] C. Chmelik, H. Bux, J. Caro, L. Heinke, F. Hibbe, T. Titze, and J. Kärger, Phys. Rev. Lett. 104 (2010) 085902.
[11] T. Titze, C. Chmelik, J. Kullmann, L. Prager, E. Miersemann, R. Gläser, D. Enke, J. Weitkamp, and J. Kärger, Angew. Chem. Int. Ed. 54 (2015) 5060.

Special Session 3
GRAIN BOUNDARIES AND INTERFACES: STRUCTURE, THERMODYNAMICS AND DIFFUSION PROPERTIES (SS3)

DSL088
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Electrochemical Chracterisation of the MmNi3.55Mn0.4Al0.3Co0.75-xFex (x = 0, x = 0.15, x = 0.35, x=0.55 and x = 0.75) Intermetallic Hydrides

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The AB5 hydrogen storage alloys such as LaNi5-based AB5 alloys can absorb and desorb a large amount of hydrogen in alkaline KOH solution when used as negative electrode in Ni-MH batteries. In this paper the electrochemical properties of MmNi3.55Mn0.4Al0.3Co0.75-xFex (x = 0, 0.15, 0.35, 0.55 and 0.75) intermetallic compounds were investigated using Chronopotentiometry, Chronoamperometry (CA) and Cyclic Voltametry (CV) techniques. The maximum electrochemical discharge capacity decreases from 260 to 200 mAhg-1 when the iron content "x" increases from 0 to 0.75. This decrease was explained by the corrosion of the alloy in the aqueous KOH solution. The hydrogen diffusion coefficient, determined by CV technique, ranges between 10-9 and 10-10 cm2 s-1. The sphere radius of particles participating in the electrochemical reaction, determined by CA technique, is about 12 μm. The obtained results are comparable to those reported in the literature.

Keywords: intermetallic hydrides, electrochemical and thermodynamical properties.

DSL328
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Grain Boundary Intermixing in Au/Ag Thin Film System and Nanoscale Kirkendall Porosity Formation

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The grain boundary intermixing in Ag/Au thin film system was studied at low temperatures (120-200 oC) for different times. The samples were prepared by DC magnetron sputtering and the composition depth profiles were estimated by means of secondary neutral mass spectrometry. Clear experimental evidence is provided by TEM on nanoscale Kirkendall porosity formation along grain boundaries and triple junctions in Ag during intermixing, where the bulk diffusion processes are completely frozen out. The porosity formation was suppressed by application of 100 bar pressure. The interdiffusion leads to homogenization in both the Ag and Au layers up to levels corresponding to compositions left behind the moving boundaries during grain boundary diffusion induced grain boundary motion, DIGM. The homogenization corresponds to saturation at certain levels (Ausat1 and Agsat2 in Ag and Au. respectively), less than 50% as predicted by the Balluffi-Cahn model [1]. It is illustrated that this saturation, during cold homogenization by DIGM, is due to stresses accumulated by the process itself: heat treating the freshly deposited Ag(Ausat1)/Au(Agsat2) films further homogenization takes place.

[1] R.W. Balluffi, J.W. Cahn, Acta Metall. 29, 493 (1981).

DSL382
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Diffusion and Solid State Reactions in Pd-Cu Thin Film Systems at Low Temperatures
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Diffusion and solid state reactions were investigated in Pd-Cu nanocrystalline films by means of SNMS (Secondary Neutral Mass Spectrometry) depth profiling technique and XRD. The heat treatments were made at such low temperatures where the volume diffusion was frozen out (150oC-310oC). At short annealing times there is a simple grain boundary interdiffusion filling up the grain boundaries. In the Pd layer, from the evolution of C-type depth profiles, the Cu grain boundary diffusion coefficients were calculated at different temperatures. At longer times first a Pd plateau developed inside the Cu. Later on the Cu penetration was also more and more extended in the Pd, even the average composition of Cu in Pd becomes higher than the average Pd composition in Cu. Although no phase formation (with interfaces parallel with the original contact plane) can be observed in the SNMS profiles, XRD patterns indicated the formation of intermetallic phase(s). Thus the overall increase of the laterally averaged compositions inside the films was attributed to grain boundary diffusion induced solid state reactions, during which the new phases grow with interface motion perpendicular to the original grain boundaries. The interface velocity in the Cu layers was estimated from the linear increase of the average composition of Pd and its value is about 1 nm/h at 220oC. The type of the growing phase depended on the ratio of the initial thicknesses and on the type of substrate.

DSL395
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Investigating the Effects of Grains Orientation and Length Scale at Crack Tip on Dislocations Activity
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In this paper, the size effects at different grain orientations are analyzed for investigating the grain behavior at crack tip. The objective of this paper is imposing the RVE to a physical strain which is produced at crack tip. Employing a strain gradient plasticity into finite element model, the enhanced description of the grains and GBs (grain boundaries) interaction is considered. The grains interaction is modeled by the modified version of the isotropic Nix and Gao theory. The plastic strain rate is initially set to be zero at interfaces to account for their impenetrability to dislocations. Increasing the stress levels, the constraints can be suppressed and grain boundary relaxation mechanism is begun. This response produce strain gradient field near the interfaces to study effect of this quantity on crack behavior. To this end, different simulations for studying dislocations activity and grain orientation were performed. It is anticipated that different crack propagation will be occurred due to grains orientation and dislocations density. Increasing the length scale related to GNDs (geometrically necessary dislocations) could change the fracture pattern. This mechanism helps to predict dislocations activity and explains an observed crossover from intergranular to transgranular fracture due to growth of the GNDs sources.

Keywords: Pile up dislocation, Size effect, Strain gradient plasticity, Interfaces at crack-tip.

DSL407
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Influence of Interface Composition on the Palladium-Germanide Formation Sequence

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The continuous down scaling of microelectronic devices aims to decrease device production cost, improve device performances, and increase the number of potential applications (miniaturization). However, this down scaling progressively leads to silicon (Si) physical limitations, similar to the case of Si oxide that has already been replaced by high-k dielectrics in current transistor production. Germanium (Ge) is another important group IV semiconductor, presenting higher charge carrier mobility and smaller band gap. This material should conveniently replace Si, particularly due to its compatibility to the Si complementary metal oxide semiconductor (CMOS) technology. Silicides are currently used as contacts in the Si-based technology. They are often produced by solid state reaction between Si and a metallic thin film using the self-aligned silicide process in the CMOS technology. Similarly, metallic contact production for the Ge-based technology needs to be investigated. Palladium germanides were shown to be interesting candidates for microelectronic applications, due to the formation of low resistivity phases at low temperature [1].

In the present work, the reaction between a 30 nm-thick Pd film and an Ge(100) substrate is investigated using in situ X-ray diffraction (XRD) and ex situ atom probe tomography (APT) analyses. In particular, this work is focused on the influence of interface initial composition on Pd germanides phase sequence formation. These results will be discussed by kinetics phenomena.

[1] S. Gaudet, C. Detavernier, A.J. Kellock, et al, J. Vac. Sci. Technol. A 24 (2006) 474

VIP008
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The State of Grain Boundaries and Grain-Boundary Diffusion in Ultrafine-Grained Mo Obtained by Severe Plastic Deformation

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The state of grain boundaries (GBs) and GB diffusion in ultrafine-grained (UFG) Mo obtained by severe plastic deformation (SPD) have been studied by the emission Mossbauer spectroscopy and radioisotope serial-sectioning analysis. The SPD was performed by high pressure torsion (HPT) by 5 revolutions of anvils at 380°C. The samples after HPT were disks of 10 mm diameter and 0.35 mm thickness, their average grain sizes being 0.45 mm in the central parts of disks (in the radius of 0.5 mm) and 0.22 mm in the periphery (at about 3.5 mm from the center). The Mossbauer studies have shown that the state of GBs in UFG Mo markedly differs from that of recrystallization grain boundaries in coarse-grained Mo. The GB diffusion coefficient for Co in UFG Mo at 350°C appeared to be several orders of magnitude higher than in case of the coarse-grained Mo with GBs of recrystallization origin, which confirms the non-equilibrium state of GBs in the former.

According to the Mossbauer data, at annealing higher than 400°C a part of grain boundaries undergo recovery and migration by short distances (the straightening of boundaries). The diffusion studies have shown that in the temperature range of 400-600°C there are two types of the accelerated diffusion paths which apparently correspond to the initial non-equilibrium GBs, formed under SPD, and to the GBs which had undergone transformations.

Beginning from 600°C there are practically no more initial non-equilibrium boundaries formed at HPT.

VIP029
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Grain Boundary Diffusion and Nanometric-Film Reaction

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The knowledge of atomic transport (kinetic and mechanisms) in nanostructured materials is of high interest for understanding, predicting and modeling nanostructure fabrication processes as well as nanostructured material ageing. The case of nanometric-film fabrication via reactive diffusion is particularly interesting since reactive diffusion processes are used in a wide range of technological applications (corrosion of metals, electrical contact fabrication on semiconductors…). During the reaction of a nanometric film with a substrate a new compound nucleates at the film/substrate interface and grows thank to interfacial reaction at the two interfaces film/compound and compound/substrate. In general, the new compound layer is polycrystalline, exhibiting nanometric (nano) grains due to the thickness of the film being in the nano-range. Thus, during the compound growth, atoms from the film and the substrate diffuse in a nano-crystalline layer made of nano-crystals (nano-grains) and mobile nano-interfaces (grain boundaries and triple junctions) under the influence of interfacial reaction. This talk will focus on atomic diffusion in Si-based nanostructures. Nano-effects on atomic transport in nanocrystals, nanometric grain boundaries (GB) and triple junctions, and the effect of GB migration on atomic transport of impurities segregating in nano-GBs will be addressed with the experimental studies of Ge [1-2] and B [3] diffusion in nano-crystalline Si [1-2], before to discuss the influence of interfacial reaction on diffusion, considering the experimental study of Si and Pd diffusion in Pd2Si during the reactive diffusion of a 30 nm-thick Pd film with a Si(001) substrate [4].

[1] Portavoce A., Chai G., Chow L., Bernardini J., Journal of Applied Physics 104, p. 104910, 2008
[2] Portavoce A., Chow L., Bernardini J., Applied Physics Letters 96, p. 214102, 2010
[3] Portavoce A., Scripta Materialia xxx, p. xxx, 2014 (see online)
[4] Portavoce A., Hoummada K., Dahlem F., Surface Science 624, p. 135, 2014

DSL332
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The Effect of Differences in the Diffusion Coefficients of Components on the Onset of Convection in Isothermal Multicomponent Systems

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The intensity of the heat and mass transfer in multicomponent systems, as a rule, is determined by molecular, convective and sometimes combined action of these modes of transport. Thus practically not taken into account the fact that even in the extreme, isothermal case, the process of molecular diffusion in liquids (vapour or gas) can lose stability, followed by the appearance of natural convection, which significantly intensifies the overall mass transfer. The instability of mechanical equilibrium is due to the difference in interdiffusion coefficients of components, which leads to a subsequent density mixture inversion that is the cause of convection in the gravity field. The paper presents the experimental and calculated data on the diffusion transfer and occurrence of convection in multicomponent mixtures.

There have been studied the isothermal diffusion of aqueous solution of three parts of salt and one part of the sugar (ρ = 1.057 g/cm3), in an aqueous salt solution (ρ = 1.125 g/cm3). Diffusion can take place till 5 s. Then there is the instability of mechanical equilibrium of the mixture. Shadow pictures have registered the convective flows that are not typical for the diffusion. Mutual diffusion in the gas mixture 0.5673 H_2 + 0.4327 Ar – N2 showed a similar pattern. For the system 0.5504 CH_4 + 0.4496 Ar – N2 convective instability was not observed. In this system the diffusion coefficients of components are comparable one to another. Consequently, the occurrence of concentration convection is only possible in systems where the diffusion coefficients of the components greatly differ from each other. The emergence of isothermal convection is connected with the problems of stability of mechanical equilibrium for the thermal convection. Spreading the formalism of the theory of stability on isothermal case there can be determined the boundaries of change of diffusion and convection modes. Comparison with experiments showed satisfactory agreement.

VIP006
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Investigation of the Saturation Effect in Solute Grain Boundary Diffusion: LMC Approach

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It is well-appreciated that, in general, for real materials the segregation of impurities is more complicated than is usually assumed for the very dilute limit that should be treated only as a convenient reference point. In this paper, we analyse the solute grain boundary (GB) saturation problem in a diffusion experiment context by means of the computer simulation technique of Lattice Monte Carlo (LMC) with constant tracer source initial/boundary conditions. This recent technique has been successfully used on numerous occasions, e.g. [1], for the purposes of systematic studies of the grain boundary transition regimes that occur between the principal well-defined Harrison grain boundary kinetics regimes (A, B and C-types). As a preliminary test case, we show that for the parallel slab model and the dilute impurity limit, the LMC simulations follow the well-known closed form solutions by Whipple [2] for the constant tracer source which in general promotes saturation. (We should note that the same applied for the closed form solution by Suzuoka [3] for the instantaneous source). Therefore the use of the LMC numerical technique is very valuable. It adds significantly to gaining an in-depth understanding of complex diffusion phenomena such as the GB saturation effect.

[1] I.V. Belova, T. Fiedler, N. Kulkarni and G.E. Murch, Phil. Mag., 92, p.1748 (2012).
[2] R.T.P. Whipple, Phil. Mag. 45, p. 1225 (1954).
[3] T. Suzuoka, J. Phys. Soc. Japan, 19, p 839 (1964).

VIP007
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Deformation-Induced Mass-Transfer during High Pressure Torsion

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The influence of high pressure torsion (HPT) on the formation and decomposition of solid solutions in several Cu-based alloys was studied. For this purpose several the Cu-based alloys with a concentration of a second component close to the maximal solubility at eutectic temperature Te were manufactured. These alloys were annealed (1) at high temperature close to Te where all (or almost all) atoms of a second component are solved in the Cu-rich matrix and (2) at relative low temperature where almost all atoms of a second component were precipitated in form of a particles of a second phase surrounded by an almost pure Cu-matrix. Such samples were subjected to the HPT at 5 GPa, 5 rot. 1 rpm. The steady-state value of the torsion torque is reached in the studied Cu alloys already after 1.5-2 anvil rotations. The precipitates in samples (2) partially dissolved in the matrix during HPT. The solid solution in samples (1) partially decomposed. Both processes proceed extremely quickly. Various mechanisms of SPD-driven mass-transfer are discussed. The resulted concentration of a second component after HPT was almost the same in samples (1) and (2). In other words, the equifinal state is reached during HPT. The composition of Cu-matrix in this equifinal state is equal to that which can be reached in equilibrium after long annealing at a certain temperature Teff. The Teff (called effective temperature) is different in different Cu-based alloys. Teff increases in the raw In à Ag à Co à Cr à Hf. In other words, Teff increases with increasing activation energy of diffusion of a second component of its melting temperature.

VIP028
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The Interface Role in the Nanomaterial Behavior at Extremes

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The notion of "extremes (extreme conditions)" as applied to nanomaterials has the special features compared with usual substances. It is well known that practically all nanomaterials are far from the equilibrium state, because many factors (the presence of numerous boundaries, triple and quaternary junctions, residual stresses, segregations, and non-equilibrium phases) give some adds into the Gibbs free energy. It is evident that under thermal, deformation, radiation, and corrosion actions (i.e. under extreme conditions) there can and must proceed many various processes including segregation, homogenization, relaxation, etc. As will shown below the nanomaterials (namely by virtue of their structural features) under extremes can be both more and less stable as compared with the usual coarse-grained analogs. The situation is non-trivial one for the presence of many various and discrepant results demanding both analysis and generalization. Current developments in the metallic nanomaterial stability under thermal, irradiation, deformation, and corrosion actions are generalized and discussed in detail. The special attention is taken to a possible prediction of the thermal grain growth characteristics using the regular solution approximation. The key role of nanotwinned interfaces in the stability increase at extremes is described and pointed out. The attention is paid to unresolved and insufficiently studied problems. Some related questions have been described in review [1].

[1] R.A. Andrievski, J. Mater. Sci. 49, 1449 (2014).

VIP051
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Interdiffusion along Grain Boundaries – Cold Homogenization of thin Films

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Unified treatment of macroscopic description of grain boundary interdiffusion is offered at low temperatures where the bulk diffusion is completely frozen out. It is assumed that diffusion induced grain boundary migration (DIGM) is a natural way of relaxation of stresses, evoked by the inequality of grain boundary fluxes. The expressions for the boundary velocity and the composition left behind the moving boundaries are related to the corresponding relations obtained by Balluffi and Cahn (Acta met. 29 (1981) 493) from a microscopic model based on climb of grain boundary dislocations. It is illustrated that, if the grain radius is less than a typical migration distance of grain boundaries, during homogenization of bilayered thin film structures forming solid solutions the system evolves to saturation with different compositions on the two sides of the diffusion pair. The composition is higher on the side of the higher melting point component. On the other hand in binary systems with compound formation grain boundary diffusion induced reaction layer formation (GBDIREAC) takes place and the final state of cold homogenization is determined by the composition of the possible intermediate phase(s) and depends on the initial thickness ratio in the film.

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VIP063
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Concentration Dependence of Grain Boundary Diffusion

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Keywords: grain boundary diffusion, concentration dependence, copper, aluminum.

There are some contradictory data about effect of alloying on grain boundary diffusion (GBD). In some systems GBD decreases with addition of impurities or alloying elements, in other - increases. GBD being very sensitive to both grain boundary (GB) structure and to interatomic interaction can be a tool to understand the processes at GB. Knowing the effect of interaction the changes in GB structure can be fixed. The some experimental results including Cu GB diffusion in so-called B regime in Al-based alloys (Al-Cu, Al-Ce) will be discussed.

Special Session 4
ALTERNATIVES ENERGY (SS4)

DSL101
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Hydrogen Storage Properties of Mg-based Alloys Prepared by HCS+MM

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Mchanical milling (MM) has been developed to accelerate the hydriding/dehydridng kinetics of Mg-based materials with nanostructures and large specific surface areas. Apart from MM, hydriding combustion synthesis (HCS) has been regarded as an innovative method to produce Mg-based hydrogen storage alloys. In our previous study, a novel nanostructured magnesium-based material with improved hydriding properties was prepared by the process combining HCS with MM [1-2]. Considering that Nano-nickel/MWCNT contains nanosized nickel uniformly distributed on MWCNT which may have a better enhancing effect on the hydrogenation and dehydrogenation of MgH_2, we have studied the HCS+MM- Mg99Ni+Nano-nickel/MWCNT system to investigate the role of joint milling of MWCNT and nanosized nickel on hydrogen storage properties of the HCS product of Mg99Ni. The effect of Nano-nickel/MWCNT on the hydrogen storage properties of HCS-Mg99Ni was investigated. It has been shown that the HCS+MM-Mg99Ni+Nanosized-nickel composite exhibits much better hydriding/dehydriding kinetics. Also the addition of MWCNT in the shape of Nano-nickel/MWCNT can further improve the hydrogenation/dehydrogenation performance. About 6.79 wt.% of hydrogen can be absorbed within 80 s at 373 K and around 97.2 % hydrogen can be desorbed within 1800 s at 543 K under initial hydrogen pressure of 0.005 MPa from the HCS+MM-Mg99Ni+Nano-nickel/MWCNT composite. This composite also exhibits an excellent cyclic stability of high hydriding rate at 423 K. In addition, the dehydrogenation activation energy of this system is reduced to 105 kJ/mol, probably ascribing to the synergetic effect of nanosized Mg_2NiH_4 and MWCNT.

[1] H. Gu, Y.F. Zhu, L.Q. Li, Mater. Chem. Phys., 112: 218-222 (2008).
[2] D.M. Liu, Y.F. Zhu, L.Q. Li, Int. J. Hydrogen Energy, 32: 2455-2460 (2007).

DSL410
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Preparation and Characterization of Cu2ZnSnS4/Se4 materials for Photovoltaic Applications

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Cu2ZnSnS4/Se4 (CZTS/Se) is a compound that shows significant potential for photovoltaic applications as absorber or counter electrode materials. This potential comes from its promising properties related to photovoltaic applications such as large absorption coefficient, having band gap of 1.4 eV to 1.5 eV, cost effectiveness, and good catalyst properties [1-3].

At this study, CZTS/Se inks were prepared via hot injection of metal precursors and sulfur source into a surfactant. Then washing and centrifuging processes were carried out to achieve pure CZTS. Different surfactants were tried to investigate the effect of surfactants to properties of CZTS. After preparation of CZTS inks, they are spin coated onto both soda lime glass and Mo coated glass. Then CZTS films were annealed at 350 C at 1 h in N2 atmosphere to eliminate the residual surfactant in the structure. CZTSe films were made via selenization of CZTS films under

N2 atmosphere at different temperatures and times to reach maximum deposition efficiency of selenium into the CZTS film structure. Then both CZTS and CZTSe films were characterized via X-ray diffraction, EDS analysis, scanning electron microscopy, surface profilemeter, Raman spectroscopy to investigate the structures, morphologies, topographies of the prepared films.

[1] Katagiri, H. Thin Solid Films,426, 480-481, (2005).
[2] Katagiri, H.; Saitoh, K.; Washio, T.; Shinohara, H.; Kurumadani, T.; Miyajima, S. Sol. Energy Mater. Sol. Cells, 65, 141 (2001).
[3] W. Wang, M. T. Winkler, O. Guanawan, T. Gokmen, T. K. Todorov, Y. Zhu, D. B. Mitzi, Adv. Energy Mater., 4, 1301465 (2014).

DSL411
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Combustion Analysis of a Direct Injection Diesel Engine with Hydrogen-Natural Gas Assisted

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Alternative fuel for internal combustions engines is one of the solutions to the limited reserve of crude oil worldwide towards the realizations of cleaner energy for sustainable future. Compared to conventional fuels use in the combustion process of engines, alternative fuels is better and cleaner because it minimize gases exhaust during combustion process of engine.

In order to achieve lean-burning capability of engines with high thermal efficiency, natural oil needs to be mixed with a fast lean-burning velocity fuel. Hydrogen is used to cut down the emissions as well as the heat loss. The ratio of natural oil and gas is variable, ranging from 0% up to 30% and the mixture of hydrogen-methane has 15-20% of hydrogen in its component. This has been a constant theme of study for researchers who studied the reaction of hydrogen with natural gas, considering the engine emission and performances. The study of the effects of adding hydrogen in compression ignition engines found out that it can widen the area of the engine operation.

The aim of this study is to investigate the combustion characteristics such as temperature, enthalpy, power and local heat flux in a direct injection diesel engine with alternative fuels assisted such as methane, hydrogen and compressed natural gas. Variables such as air mass flow rate, temperature, pressure and the type of fuel were used to study the heat loss that occurs in the combustion chamber. This study was conducted through computer simulation method by using the computational fluid dynamics software ANSYS Fluent.

DSL415
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Preparation and Characterization of Activated Carbon from Diss and Esparto Grass by Chemical Activation with KOH and Zncl2

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Esparto (Alfa is the Arab name for esparto) and diss grass have been used as new raw lignocellulosic materials to obtain activated carbons using zinc chloride ($ZnCl2$) and potassium hydroxide (KOH) as activating agent. The technical activation at 650°C under nitrogen atmosphere was studied in this work. The microstructures and microcrystallinity of the activated carbons prepared were examined by scanning electron microscope (SEM), energy dispersive analysis of X-rays (EDX), and powder X-ray diffraction (small-angle X-ray scattering) techniques. The apparent surface area was estimated by nitrogen adsorption (BET). The results showed that the surface area and pore volume of activated carbons have achieved their highest values 989m²/g and 0.375cm3/g, respectively. These experimental results indicated the potential use of esparto and diss grass precursor in the activated carbon preparation process.

In a second step we discussed the basic principles of acquisition and image processing: Techniques approaches by conventional geometric shapes (circle, ellipse ..). For structural analysis: length, tortuosity, curvature, orientation, skeletonization.

Keywords: Activated carbon; structural analysis, image processing

VIP009
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Development of Ecoefficient Alternatives for the use of Hydrogen as Energy Carrier using Smart Materials

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The weaknesses of the current energy model, mainly based on fossil fuels, and the need of reducing the CO2 equivalent emissions to meet new legal requirements, have promoted the interest in developing alternative ways of obtaining energy. Although the use of renewable energy is essential to achieve a "zero emissions economy", there are many technical and practical limitations which need to be overcome. On the one hand, renewable energy sources are usually intermittent, so they require a storage system to ensure a continuous supply. On the other hand, nowadays, more than the 70% of the total primary energy consumption takes place in combustion processes, so the substitution of all the combustion plants by renewable energy is not possible, at least in the medium-term. Consequently, a first step towards the low carbon energy is the improvement of the current combustion plants to adapt them to the use of cleaner fuels. In particular, the use of hydrogen is considered one of the most promising alternatives.

Although hydrogen can be used in widely different processes (combustion, fuel cells…), all the alternatives require a storage stage. However, despite being a critical stage for the implementation of a global hydrogen economy, there is an important lack of agreement about which is the best method to develop an efficient, reliable, safe and economically viable method of storage.

For that purpose, the storage of hydrogen in solid systems has been considered the most reliable methods in the long term. However, many technical problems, such the demand of energy during the storage or the storage capacity, must be solved during the next few years. In order to face up to these problems and propose practical solutions, CIRCE is working on the development of a novelty and ecoefficient alternative focused on taking

advantage of the use of phase change materials to reduce the energy consumption in the storage process, which, at this moment, is one of the main drawbacks of the solid storage.

DSL093
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Application of Multicriteria Method on Alternative Energy Selection

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There are many forms of alternative energy, such as: the biomass energy, geothermal energy, hydraulic energy, wind power and solar energy.
Each form has its natural characteristics and its own exploitation conditions, thus, the choice of the best resource does not depend only on provided energy capacity but also on other criteria.

For this reason, our survey applies the multicriteria method to classify these energy resources based on several criteria.

Keywords:
Alternative energies, multicriteria method, technical and operational conditions

DSL210
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Hydrogen Behavior in NdRh3-Based Hydrides

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Intermetallic compounds (IMC) RTx (R-rare earth metal, T-d-metal, x-2, 3, 5) are able to absorb reversibly large amount of hydrogen and are materials for it safety storage [1]. In work [2] was revealed that interaction of NdRh3 (CeNi3 hexagonal structure type) with hydrogen under high pressure (up to 2000 bars) leads to formation of hydride phase having lattice with cubic AuCu3 structure and ordered hydrogen. In [3], using neutron powder diffraction method was determined hydrogen atoms location in the lattice of CePd3 and CeRh3 hydrides with AuCu3 structure. This work presents results of the study of NdRh3 hydride samples having coexisting together two phases with hexagonal and cubic lattices and obtained after hydrogen desorption at high temperature. It was revealed that depending on $\partial t0C/\partial t$ (t0C is temperature, t is time of heating) conditions the proportion of these two phases in the hydride samples changing broadly. The explanation of this is proposed on base of different diffusion of ordered hydrogen in the cubic lattice and disordered hydrogen in the hexagonal lattice. Ordered hydrogen atoms charged partly negatively ($H\delta$-), have slow diffusion and it is favourable for formation of phase with cubic lattice. Disordered hydrogen atoms charged partly positively ($H\delta$+), have fast diffusion and this leads to decrease phase with hexagonal lattice in the hydride sample. Varying the rate of $\partial t0C/\partial t$ during desorption of hydrogen, it is possible to change amount of phases with hexagonal and cubic lattices in the hydride samples.

[1] M.Latroche and A.Percheron-Guegan, J. Alloys and Compound, 356-357, 461 (2003).
[2] S.A. Lushnikov, T.V. Filippova, K.M. Podurets and A.V. Gribanov, Inorganic Materials, 47-3, 240 (2011).
[3] H. Kohlmann, F. Muller, K. Stowe, A. Zalga and H.P.Beck, Z. Anorg. Allg. Chem., 635, 1407 (2009).

DSL230
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Energy Model Applied to Renewable Energy in Housing Systems

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In recent decades, global events and extreme changes make sustainable development and renewable energy a frequent subject of discussion in numerous global meetings. To analyze the energy matrix of a region in order to optimize it sustainably is a way to reduce their impacts. Currently, the world energy matrix is made up of 81.0 % of non-renewable sources, namely: 78.4% oil and oil products, natural gas and coal, 2.6 % uranium, and 19.0 % from renewable sources, distributed in: traditional biomass 9.0 %, Bio-heat 2.6 %, 3.8% hydropower and others renewable energies 3.6 % (solar, wind, geothermal, biodiesel, ethanol, ocean power, etc.). Energy is defined as the amount of work that a physical system is able to perform [1], so, we seek to take advantage of using the most of these sustainable and renewable resources [2]. Regarding renewable sources emphasis is related to solar and wind power to produce electricity.

In this sense, the aim of this work is to establish a sustainable model of energy planning in a region taking into account local characteristics and the efficiency in the power generation for residential systems. Were collected energy demand data in different Brazilian companies. From the data obtained, it was found that the method / model used is very efficient for the case study related to energy efficiency of housing systems using renewable energy.

[1] G. J. Van Wylen, R. E. Sonntag, C. Borgnakke, Fundamentals of Classical Thermodynamics. London: John Wiley & Sons, Inc. (1993).
[2] J. Goldemberg, O. Lucon, Energy, Environment and Development. 3.ed. São Paulo: Editora da Universidade de São Paulo (2008). (In Portuguese)

DSL233
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Coupled Photon-Electron-Phonon Transport inside Metallic Nanoparticles Enhanced Thin-Film Solar Cells

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The world is blessed with abundant of solar energy throughout the year. Not only this serves as an unlimited renewable-energy reservoir, but also it presents an opportunity for all of us to be living in a clean and sustainable

environment for centuries to come. Harvesting the solar energy is usually done through the use of solar cells, which is basically a p-n junction or multiple junctions stacked together. Traditional solar cells rely on the material volume to generate as many electron-hole pairs as possible and convert solar energy to electricity. However, such devices are typically expensive due to the high manufacturing costs. On the other hand, thin-film solar cells (TFSCs) are great substitutes for traditional crystalline and bulky solar cells because of low production cost, although their efficiencies are lower in comparison. Efficiencies of TFSCs can be enhanced using metallic nanoparticles; however, a thorough account for combined electrical and thermal analysis for this application is still missing. This is crucial in order to fully take advantage of these nanoparticles in enhancing conversion efficiency. The main aim of this work is to analyze the efficiency enhancement of thin-film solar cells due to embedded metallic nanoparticles from both electrical and thermal aspects. The nanoparticles present deep inside the cell reflect incident radiation which then increases the optical path length for enhanced electricity generation. The increase in the optical path length also tends to induce additional but undesirable thermal heating which reduces the performance of the cells. The relationship between the improved conversion efficiency and the thermal effect is the crucial factor of maximizing the performance of thin-film solar cells and has yet been explored. An accurate theoretical/numerical modeling is warranted in this case. Here, we will present and outline details of various thermal transport mechanisms involved in the cell with the inclusion of semi-ballistic effect. Some preliminary results will also be discussed.

DSL245
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Study of Pollutant Emissions of Diesel Engine Operating with Mixture of Diesel, Biodiesel and Natural Gas

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Fossil fuels are in continuous process of reduction. Find alternative fuels to reduce emissions of pollutants, it is necessary. Biodiesel is one of the best renewable resources available that have appeared recently.
The gaseous fuel used in engines of the diesel cycle has been much studied in recent years, due to the characteristics positive of these fuels when the focus is the level of emissions launched in the atmosphere.
The challenge is to transform the engine diesel into dual engine by using adequate mixtures of diesel, biodiesel and natural gas to obtain correct ratio of each fuel and to maintain the original characteristics of diesel engine and good performance[1,2].
In this sense, the objective of this research is to study the emission characteristics of a commercial diesel engine working with biodiesel (B20, B30 and B40) and natural gas mixture. The fuel used in motor consists of 15% mixture of diesel and biodiesel (liquid fuel) and 85% natural gas; experiments were carried out in powers 80, 100 and 120 kW. The engine was instrumented in order to obtain temperature, mass flow rate, pressure and concentration of combustion gases during the experimental test. From the experimental results it was verified that NOx, NO, and CO_2 concentrations decrease. It was also verified an elevated reduction on level the emissions of these exhaustion gases compared to diesel standard.

[1] Y. J. R. Costa, A. G. B. Lima, C. R. Bezerra Filho, M. B. Grilo, A. M. N. Lima., Braz. J. Petrol. Gas. 2, 36-44, (2008)
[2] A. E. Atabani, A. S. Silitonga, I. A. Badruddin, T. M. I. Mahlia, H. H. Masjuki and S. Mekhilef: Sust. Energ. Rev.16, 2070-2093,(2012).

DSL296
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Three-Dimensional Morphology Analysis of Fuel Cell Catalysts for the Numerical Comparison of the Effectiveness between Conventional and Vertically Aligned Carbon Nanotube Electrodes

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The effectiveness of conventional and vertically aligned carbon nanotube (VACNT) electrodes are estimated by statistical three-dimensional morphology analyses. Multi-phase random structures of cathode catalyst layer (CCL) in PEFCs were reconstructed and simulated by imitating the procedure of membrane electrode assembly (MEA) preparation. In this present study, various compositions, including Pt/C volume fraction and ionomer contents, and morphological structures of CCL, such as conventional and VANCT electrodes were simulated to elucidate the effect of gas diffusion and electron/proton conducting pathways on the effectiveness of Pt/C electro-catalysts. Each set of random samples was generated over a representative elementary volume domain to satisfy a 95% confidence level for in-depth statistical analysis. The statistical morphology analyses reveal distinct increasing tendency of effectiveness with increasing ionomer contents. For the conventional electrodes of 32vol.% Pt/C, the optimal composition of catalyst layer was predicted as 31vol.% of ionomer corresponding to 37% of porosity with the maximum effectiveness value of 28.7%. Additionally the VACNT electrodes of 30vol.% of Pt/CNT were found to have drastic improvement in effectiveness with statistical maximum value of 39.8% at optimal composition of 34vol.% of ionomer. We conclude that the improved electron conducting pathways due to morphological structure of VACNT electrodes can lead more efficient fuel cell MEAs. This statistical three-dimensional morphology analysis for fuel cell catalyst electrode enables us to gain a priori insight into the morphological effects of various catalyst configurations on the effective transport properties and electrochemical reactions in fuel cells.

VIP010
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Dimensional Analysis and Modelling in Thermohydrodynamics of Two-Phase Flows

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Dynamics and heat and mass transfer in typical for the current energy systems gas-liquid systems with phase change are the most challenging problems in thermofluids. Variety of changing with time flow patterns, wavy effects at the interface, complicated turbulent transfer due to phase interaction, strong effect of geometrical characteristics of equipment do not allow the development of comprehensive and detailed theoretical analysis and lead to expensive experimental studies. In this connection the dimensional analysis becomes an efficient and important tool for the processing of experimental data and the mathematical model development at an initial stage.

The first class of gas-liquid flow problems discussed in the lecture is related to the construction of the regime map for rising gas bubbles. Traditional approach of using external length scales does not allow the efficient generalization of many known factors. The use of the inner characteristic scales related to the interaction of the external fields and surface effects $\delta_v=[v^2\rho_L/g(\rho_L-\rho_G)]^{1/3}$ and $\delta_\sigma=[\sigma/g(\rho_L-\rho_G)]^{1/2}$ as a reference frame ($R_v=R/\delta_v$, $R_\sigma=R/\delta_\sigma$), allows representation of every medium by the straight-line, whose slope does not involve the bubble rising velocities and depends on the Morton number $Mo=\rho^3v^4g/\sigma^3=(\delta_v/\delta_\sigma)^{1/6}$. Thus, the map of bubble rising

regimes enables, besides the self-similar limiting cases, to calculate the bubble rising velocity in the intermediate regions.

The key to our approach for the second class of gas-liquid flow problems, hydrodynamic theory of heat transfer in boiling, lays with dimensional analysis and scaling of high turbulence intensity in the near-wall zone and intensive local acceleration due to the bubble departure suggesting structural similarity of the near-wall zone of boiled and injected liquid. Gas compression into a bubble appears as a governing hydrodynamic factor. The limiting heat transfer law takes the form, $Nu = const\ Re^{2/3}Pr^{2/3}M^{-4/3}$, where criterion M takes into account pressure effect on transfer processes in boiling and gas injection. Conceptually this law is more universal than previously proposed models.

DSL243
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Synthesis and Characterization of Cu2ZnSnS4 Absorber Layers by Ultrasonic Spray Pyrolysis

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Keywords- CZTS, spray technique, thin films, photoluminescence, Transmission, XRD, electrical conductivity.

The influence of substrate temperature on the properties of Cu2ZnSnS4 thin films elaborated by spray ultrasonic method has been investigated. Samples are deposited at various substrate temperature ranged from 280 to 360 °C about 45 min. the results of X-ray diffraction analyses indicated that Cu2ZnSnS4 films have nanocrystalline structure with (112) preferential orientation and reveals the formation of ZnSnO3 and Cu2ZnSnS4 phases. The crystalline size is varied from 20 to 45 nm with increasing substrate temperature. The optical films characterization was carried out by the measurement of UV-visible transmission. The optical gap was deduced from the absorption spectra. The photoluminescence spectrum measured at 77 K showed a broad emission around 1.27 eV. Electrical conductivity of the films is found to lie in the range 9 to 43 (Ωcm)-1.

VIP011
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Band Gap and Adsorption Energy Evaluation of Magnetic and Haematite Supported Single Wall Carbon Nanotubes for Green Urea Production

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Keywords: Magnetic induction method, Magnetite, Hematite, Band gap, Urea

Urea has always been the most sorted synthetic fertilizer in agriculture industry. An essential need exists for an investigation of new synthesis method for production of urea under ambient conditions. This requires some effort in band gap and adsorption energy of the reactant gasses on catalyst and the support simulation to be done prior to experimental work. Experimental production of green urea using carbon nanotubes with magnetite or hematite as support/catalysts at room temperature and ambient pressure was conducted in high magnetic flux density reaction chamber. The band gap of single wall nanotubes (SWCNTs) is 0.115 eV and it involves 96 numbers of electrons. However SWCNTs with magnetite gives 0 eV band gap and 224 numbers of electrons. The lower band gap and higher number of electrons indicate increased potential of catalytic activities to take place hence higher urea formation. Further simulations show that adsorption of reactant gases resulted to band gap of magnetite to be reduced to 0.014 kcal/mol and that of hematite with SWCNTs turns out to be zero during the urea formation at room temperature and pressure. The vanishing of band gap when CNTs are dispersed on hematite makes its valence band to coincide with conduction band hence perfect conductivity which is vital for magnetic induction method. On the other hand magnetite supported with CNTs exhibits lower adsorption energy (-151.949 kcal/mol) during urea formation which is more favorable energetically. Urea, confirmed by FTIR peaks was formed in the magnetic reaction chamber with less than 2.0 Tesla and the presence of carbon nanotubes/magnetic catalysts under ambient conditions.

Special Session 5
CARBON AND OXIDE NANOSTRUCTURES (SS5)

VIP044
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Photomagnetomechanical Effect in Graphene

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This paper summarizes contactless and nondestructive photoelectromagnetic (PEM) methods of investigations of semiconductors. Such investigations allow to determine optical, transport and recombination parameters of excess carriers in the investigated materials. The PEM investigations are especially suitable in the case of semiconductors with higher carrier mobilities, e.g. in the case of graphene. The main aim of this paper is to present the photoelectromagnetic method of investigations of graphene in Corbino configuration. In this configuration the so called photomagnetomechanical (PMM) effect is observed. When a graphene sample is illuminated by a circular spot of radiation, free electrons and holes are photogenerated in the illuminated spot and diffuse in all directions in the layer. In external magnetic field with component perpendicular to graphene surface the diffusing carriers are deflected by Lorentz force and the circulating PEM current flows. The loops of a circulating current have a magnetic moment. Due to the interaction between this moment and a component of external magnetic field parallel to graphene, there is the PMM torque acting on the sample. This phenomenon allows direct transformation of light into mechanical energy. Strength of the PMM effect is strongly dependent on the mobility and diffusion length of carriers. We present results of theoretical calculations as well as experimental data obtained for graphene films deposited on different substrates.

DSL092
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Biosynthesis of Lipids from Waste of Food Industry

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During our work we have proposed to develop a substrate rich in carbon and nitrogen from waste apricot, plums and grapes. For this we bioconverted these resources through a ferment complex acting in synergy to pH = 5 and at a temperature T = 50 ° C.The hydrolysis was measured by colorimetry following the release of reducing sugars. Meanwhile we have experienced on a synthetic culture medium and 32 strains of yeast we chose four perspective wealth lipid biomass. It is: Lipomyces starkeyi; Rhodotorula gracilis; Cryptoccocus terricolus and Rhodosporidium toruloides.Aprés Correction stoichiometric ratio of carbon / nitrogen were seeded in said substrate selected yeasts, this has enabled us to follow in the biosynthesis and the time noted that this reaction follows a zero-order kinetics (Graph 1). variation conditions biosynthesis gives maximum efficiency for a pH between 5 and 6 and T = 25 ° C (graph 2).

Table No. 1
composition Group of yeast

	Lipomyces Starkeyi	Rhodotorula gracilis	Cryptoccocus terricolus	Rhodosporidium toruloides
In% fat	0.12	0.32	0.17	0.10
Diglycerides%	4.12	0.71	1.24	2.85
Fatty acids %	1.95	1.20	1.56	0.89
Triglucérides%	91.93	85.47	90.03	79.06
Iodine in %	73.7	82.90	85.40	70.09
Acid mgrKOH / gr	3.90	2.46	2.93	1.82

After solvent extraction of the fat and chromatographic fractionation yields the composition shown in Table No. 1, we note that triglycerides are the major product biosynthesis. These lipids are synthesized in the standards and can be recommended in cosmetics in the first place.

DSL264
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Effect of Agnps Decorated Microstructures Zno on the Photodegradation of MB using Zno under UV Light Irradiation

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ZnO has been widely investigated as one of the important material for photocatalytic applications due to its large initial rates of activities, having active sites with higher surface reactivity [1]. Combined with the advantages of non-toxicity, high stability, cost effective and environmental safety, ZnO has become a potential photocatalyst for remediation of environmental problem [2]. It is reported that, ZnO photocatalyst also presents some challenges such as fast recombination rate of the photogenerated electron-hole pair and low quantum efficiency, which resulting low photocatalytic efficiency reaction in the system [3][4]. Therefore, in order to improve the photocatalytic activities, researchers have been found that doping is one of the alternative ways to improve the photocatalytic properties. In this work, AgZnO nanoparticles were prepared by sol-gel method with varying the Ag concentration. The photocatalytic activities of the pure ZnO and AgZnO nanoparticles act as photocatalyst prepared by sol-gel method were studied by the degradation of methylene blue (MB) under ultraviolet irradiation.

In this work, the photocatalyst has been prepared by mixing a 5.0 g of ZnO powder with $AgNO_3$ and HMTA at 0.05 M and 0.1 M concentration in 300 ml of DI water. The mixture was then heated at 95 °C for 6 h. After completion, the obtained white-greyish precipitates was washed repeatedly with deionized water and finally dried at 300 °C for 2 h. The photodegradation measurement was carried out through the degradation of methylene blue (MB) dye in aqueous solution. 50 mg of pure ZnO, 0.05 M and 0.1 M AgNPs decorated microstructures ZnO photocatalyst were placed into a beaker containing 20 mg/L MB in 300 ml DI water and the solution then were irradiated under ultraviolet (UV) light (main wavelength: 254 nm). After irradiating for 10, 20, 30, 40, 50 and 60 minutes, the concentration of residual MB was determined by the absorption of the reaction solution at the characteristic absorption wavelength 664 nm using UV–visible spectrophotometer.

FESEM and EDX analysis for all photocatalysts have been characterized. The photocatalyst was composed of particles structure with average size of 300-500 nm. The morphology and size of the photocatalyst do not show significant changes when Ag was loaded into the ZnO. However from EDX spectra, the atomic % of Ag increased as higher Ag concentration was added with value of 5.6 at. % and 16.1 at. % for sample 0.05 M and 0.1 M AgNPs decorated microstructures ZnO photocatalyst. XRD results confirmed that all the diffraction peaks are corresponding to the hexagonal wurtzite ZnO and cubic metallic Ag crystal, respectively. No other peak was

detected and there was no significant shift for all diffraction peaks indicating that the silver didn't substitutes for Zn2+ or interstitial atom [5][6].

Photodegradation rate constant, k of different photocatalyst were observed with value of 0.016, 0.026 and 0.032 min-1 for pure ZnO, 0.05 M and 0.1 M AgNPs decorated microstructures ZnO photocatalyst, respectively. 0.1 M AgNPs decorated microstructures ZnO photocatalyst that having the highest photodegradation efficiency was observed to be the optimum concentration for enhance the photodegradation activity compared to pure ZnO and 0.05 M AgNPs decorated microstructures ZnO photocatalyst. It has been proposed that the photodegradation activity of AgNPs decorated microstructures ZnO photocatalyst is due to Schottky barrier formed between Ag and ZnO interface [7].

In summary, AgNPs decorated microstructures ZnO photocatalyst have been prepared by sol-gel method. FESEM, EDX and XRD results demonstrates that obtained photocatalyst are consist of Ag element. The photodegradation analysis shows that the 0.1 M AgNPs decorated microstructures ZnO photocatalyst exhibit a higher photodegradation activity compared to pure ZnO and 0.05 M AgNPs decorated microstructures ZnO photocatalyst. The increase of the rate constants, k in the presence of Ag was due to the prolonged lifetime of the photogenerated electron hole pairs in ZnO as a result of Ag nanoparticles acting as electron sink.

[1] C.-W. Chang, H.-T. Wu, S.-H. Huang, C.-K. Chen, I.-W. Un, T.-J. Yen, Acta Mater., 61 , 6993 (2013).
[2] S.J. Pearton, D.P. Norton, K. Ip, Y.W. Heo, T. Steiner, Prog. Mater. Sci., 50, 293 (2005).
[3] Z. Han, L. Ren, Z. Cui, C. Chen, H. Pan, J. Chen, Appl. Catal. B Environ. ,126, 298 (2012).
[4] B. Subash, B. Krishnakumar, B. Sreedhar, M. Swaminathan, M. Shanthi, Superlattice Microstruct., 54, 155 (2013).
[5] R. Georgekutty, M.K. Seery, S.C. Pillai, J. Phys. Chem. C, 112, 13563 (2008).
[6] Z. Yang, P. Zhang, Y. Ding, Y. Jiang, Z. Long, W. Dai, Mater. Res. Bull., 46, (2011) 1625.
[7] B. Chai, X. Wang, S. Cheng, H. Zhou, F. Zhang, Ceram. Int., 40, 429 (2014).

DSL265
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Fabrication and Characterization of Fe doped TiO2 Membranes for Ultrafiltration

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Fe doped TiO2 nanoparticles have been synthesized using a reverse micelle and sol- gel technique combined with metal alkoxide hydrolysis and condensation. The size of the particles and the thickness of the coating can be controlled by manipulating the relative rates of the hydrolysis and condensation reaction of TTIP within the micro-emulsion. The average size and distribution of synthesized Fe doped TiO2 nanoparticles was about in the size range of 10-20nm and Fe particles are 1-3nm. The intermediate layer of membranes was made with spherical SiO2 about 100nm. Fe doped TiO2 composite membranes were fabricated by slip casting. The FE-SEM image show the microstructure of the Fe doped TiO2 composite membranes was homogeneous. Average pore size of the support was about $0.125\mu m$ and the pore size distribution was narrow. The average pore size of the Fe doped TiO2 composite membranes have smaller than that of TiO2 composite membranes. It was observed that Fe doped TiO2 composite membranes showed a crack-free microstructure and narrow particle size distribution even after heat treatment up to 1100℃.

DSL285
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Synthesis and Characterisation of Silica Nanoparticles with Different Particle Size

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Silica nanoparticles have been used in various electrical products, cosmetics and medicine, the particle size and shape of silica influencing the quality and performance of a number of these [1-3]. Silica nanoparticles have been synthesized at room temperature using tetraethylorthosilicate (TEOS), ethanol, deionized water and ammonia solution via sol-gel technique. Fine spherically shaped silica nanoparticles have been obtained by increasing the amount of ethanol in the mixture. Using scanning electron microscopy (SEM), a high-resolution transmission electron microscope (HRTEM) and x-ray diffraction (XRD), characterization was made of the morphology and elemental composition of the nanoparticles. From the SEM images, the particle sizes for three types of sample were measured to be within the range 30-80 nm, 90-170 nm and 500-550 nm.

Reference
[1] Park, Y.-H., Bae, H., Jang, Y., Jeong, S., Lee, H., Ryu, W.-I., Yoo, M., Kim, Y.-R., Kim, M.-K., Lee, J., Jeong, J., Son, S., 2013. Effect of the size and surface charge of silica nanoparticles on cutaneous toxicity. Mol. Cell. Toxicol. 9, 67–74.
[2] Slowing, I.I., Vivero-Escoto, J.L., Wu, C.-W., Lin, V.S.-Y., 2008. Mesoporous silica nanoparticles as controlled release drug delivery and gene transfection carriers. Adv. Drug Deliv. Rev. 60, 1278–1288.
[3] Barisik, M., Atalay, S., Beskok, A., Qian, S., 2014. Size Dependent Surface Charge Properties of Silica Nanoparticles. J. Phys. Chem. C 118, 1836–1842.

DSL312
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Application of Red Mud-Based Zn/Al Oxide Catalyst for the Reaction Synthesis of Glycerol Carbonate from Glycerol and Urea

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Red mud is an abundant waste product generated in the industrial production of aluminium. It has good properties such as aluminum and iron content, high surface area, sintering resistance, resistance to poisoning and low cost [1]. This research applies red mud as catalyst for the reaction synthesis of glycerol carbonate from glycerol and urea. It's reported the high performance of Zn/Al catalyst for glycerol carbonate synthesis reaction [2]. Typically, a red mud-based Zn/Al oxide catalyst is prepared by hot wet impregnation method, followed by calcination at 450oC in 6h. The catalyst is experimented for the synthesis of glycerol carbonate from glycerol and urea in batch reactor at 140oC under vacuum condition (3kPa) to remove ammonia by-product. Products are analyzed by GC-FID using internal standard method (tetraethylene glycol). Catalyst characterizations are studied by BET surface area, XRD and FE-SEM analyses. The ratio between Zn and Al and the weight loading of metal on red mud are varied to find out the best performance catalyst.

[1] S. Sushil, V.S. Batra, Appl. Catal. B: Environ., 81 , 64 (2008). [2] M.J. Climent, A. Corma, P. De Frutos, S. Iborra, M. Noy, A. Velty, P. Concepción, J.Catal., 269, 140 (2010).

DSL359
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Elaboration and Physical Characterizations of Multiphases Nanocomposites Materials

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Carbon nanotubes (CNTs) are promising materials due to their very interesting physical and chemical properties. They are the subject of multiple applications and in particular as reinforcing agents in polymer-based composites. Multifunctionnal nanocomposites based on CNTs have attracted an extensive attention since they can provide excellent mechanical, electrical and thermal properties [1]. The improvement of these properties is based on the good dispersion of carbon nanotubes in the matrix and their interfacial interactions. Hence, the use of grown carbon nanotubes on diatoms is a challenging solution to provide a well disperse inclusions in a polymer matrix. Diatoms are natural silica which present a high specific surface area due to their naturally well-organized nanopores and nanochannels. Several techniques have been developed to form CNTs but Catalytic Chemical Vapour Deposition (CCVD) is the most widely used [2]. This method uses metal nanoparticles (Ni, Co, Fe…) as catalysts to improve the yield of CNT production.

Here we investigate the mechanical, electrical and thermal properties of nanocomposites based on Polymethyl methacrylate (PMMA) and biphased materials (diatoms+CNT) as a reinforcing agent. The growth of CNTs on diatoms was done by CCVD on fluidized-bed reactor. The catalytic nanoparticles are made by vapour phase impregnation of cobalt acetylacetonate.

The investigation of the biphased materials dispersion in the PMMA matrix has been jointly obtained by Scanning Electron Miscroscopy and Tunneling Electron Miscroscopy. The mechanical properties, electrical conductivity and thermal stability of the multiphase nanocomposite were investigated.

[1] H. Lorenz, J. Fritzsche, A. Das, K.W. Stöckelhuber, R. Jurk, G, Heinrich b, M. Klüppel, Composites Science and Technology 69 2135–2143 (2009).
[2] M. Kumar and Y. Ando, Journal of Nanoscience and Nanotechnology 10 3739–3758 (2010).

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Carbon Nanospheres for Electrochemical Applications :
Raman, FTIR and XPS Studies

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The effect of Fe-catalyst impurities on the structure of carbon nanospheres (CNSs) with diameters 50-100 nm, synthesized via direct pyrolysis process, has been investigated. The CNSs were produced in a electric furnace. The chemical bonding properties of CNSs was studied by means of X-ray photoelectron (XPS), Fourier Transform Infra Red and Raman spectroscopies. XPS studies showed a presence of a sp3 bonded carbon sites. These results were then confirmed by Raman spectroscopy that showed that the ID/IG ratio was affected by the presence of Fe-catalyst. In addition, it was shoen by the observation of transmission electron microscopy that the spheres have a turbostratic structure. The possible use of CNSs in the electrochemical fields especially as electrodes in lithium ion batteries will be the main application in our experiments.

Keywords: Fe catalyst, Carbon spheres, Raman, XPS, Bonding Properties

References
[1] H.W. Kroto, J.R. O'Brien, R.F. Curl, R.E. Smalley, C60: Buckminsterfulleren, Nature 318 (1985) 162–163.
[2] S. Iijima, Helical microtubules of graphitic carbon. Nature 3544 (1991) 56–58.
[3] O. Wohler, F.V. Sturm, E. Wege, H.V. Kienle, M. Voll, P. Kleinschmit, Ullmann's Encyclopaedia of Industrial Chemistry, Vol. A5, Gerhartz W (ed.). Weinheim: VCH, 1986.
[4] D.P. Abraham, D.W. Dees, J. Christophersen, C. Ho, A.N. Jansen, Performance of high-power lithium-ion cells under pulse discharge and charge conditions, International Journal of Energy Research 34 (2010) 190–203.
[5] A. Deshmukh, S.D. Mhlanga, N.J. Coville, Carbon spheres. Materials Science and Engineering R 70 (2010) 1–28.

DSL400

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The Comparison of Cure Behavior of Epoxy and Multi-Wall Carbon Nanotube/Epoxy Composites

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The influence of multi-wall carbon nanotube (MWCNT) on the cure behavior of epoxy (LY564) was investigated by using differential scanning calorimetery (DSC) in dynamic scan mode. The results indicated that nanotubes could initiate cure reaction at lower temperature by decreasing the peak temperature (T_p). Also, a correlation was established between the dispersion state of MWCNT in epoxy and the residual enthalpy of the partially cured resin (ΔH_{res}), where lower was considered as an indication of better interfacial interaction of carbon nanotube with matrix and hence, better dispersion. Results from activation energy method showed that activation energy of MWCNT/epoxy nanocomposites increased in comparison with that of the neat epoxy, revealing that MWCNT significantly hindered the occurrence of vitrification. Addition of 2 mass% MWCNT to the epoxy matrix caused region of curing in the glassy state, which is controlled by diffusion, become larger than that of neat epoxy. Finally, scanning electron microscopy (SEM) was applied to investigate correlation between the dispersion of MWCNT in epoxy matrix and cure behavior of samples.

DSL405

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Hydrogen Absorption Capacity of Nanostructured La0.9Ca0.1Ni5 Intermetallic Compound

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Nanocrystalline La0.9Ca0.1Ni5 intermetallic compound was produced from the elemental components by vacuum induction melting and subsequent mechanical milling. Microstructural and morphological analyses were carried out using X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM), while hydrogen absorption analyses were performed in a Sievert-type apparatus. The results showed that the 10 h milled sample had a typical nanocrystalline structure, while the 30 h milled sample displayed a mixture of nanocrystalline and amorphous structures. The lattice constants and unit-cell volume were found to decrease with increasing the milling time. Moreover, the hydrogen absorption decreased and the hydrogen absorption plateau regions narrowed with increasing the milling time. The results indicated that the emergence of nanocrystalline and amorphous phase mixture rendered detrimental effect on the hydrogen absorption capacity in the long time ball-milled La0.9Ca0.1Ni5 powders.

DSL409

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Nanocomposites Reinforced with Cellulose Nanocrystals

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In this paper was prepared cellulose nanocrystals from nanocrystals Munguba fibers (Pseudobombax Munguba). Initially the fibers have been subjected to bleaching process for the partial removal of lignin and hemicellulose by exposing the cellulose fiber and thus facilitates the acid hydrolysis. The nanocrystals were extracted from Munguba fibers by acid hydrolysis with sulfuric acid solution and 55% were modified by graphitization. These materials will be characterized by X-Ray Diffraction (XRD) to determine crystallinity index, Infrared Spectroscopy (FTIR) evaluating the chemical modification, Transmission Electron Microscopy (TEM) evaluating the morphology of the nanocrystals, contact angle and the thermal stability will be evaluated by analysis thermogravimetric (TGA). The use of modified nanocrystals resulted in improved the thermal stability of the nanocrystals, changing the polarity and crystallinity. Nanocomposites filmes was prepared and characterized by differential scanning calorimetry (DSC), scanning electron microscopy (SEM) and analysis thermogravimetric (TGA). The results showed a good dispersion of nanocrystals in the matrix, as well as its nucleating effect.

DSL204

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Formation and Growth Mechanisms of Silver Nanoparticles in Ion-Exchanged Glasses

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Irrespective of the great amount of works published in this field, the study and the control of metal nanoparticles growth in glass matrixes is still a relevant task [1-3]. In particular, the application of nanostructured glasses containing silver nanoparticles has been extended to biomaterials, solar technologies, plasmonics, catalysis, sensoristics, and in general to a wide range of specific functional systems [4]. In this work, we deal with the growth of silver nanoparticles in ion-exchanged glasses, promoted by thermal treatments in air, since the role of point defects of the glass matrix and of the temperature in this process is still to be comprehensively described. The particle dimension was measured as a function of depth by means of low-frequency cross-sectional micro-Raman measurements, which allow to detect particles of size of about 1 nm. Moreover, luminescence surface analysis were performed in order to study the aggregation state of silver below the surface. Finally, reaction-diffusion equations were integrated by means of numerical methods, to gain information on the point defect concentration effects as well as on the temperature dependence of the parameters underlying migration and reaction of the involved species.

[1] A. Quaranta, A. Rahman, G. Mariotto, C. Maurizio, E. Trave, F. Gonella, E. Cattaruzza, E. Ghibaudo, J.-E. Broquin, J. Phys. Chem. C, 116, 3757 (2012).
[2] A. Simo, J. Polte, N. Pfander, U. Vainio, F. Emmerling, K. Rademann, J. Am. Chem. Soc., 134, 18824 (2012).
[3] A.V. Redkov, V.V. Zhurikhina, A.A. Lipovskii, J. Non-Cryst. Solids, 376, 152 (2013).
[4] F. Gonella, Ceramics International, 41, 6693 (2015).

DSL216
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Microwave Conductivity of Fe based Nanocomposites

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In the present study we report on the microwave conductivity of Fe based nanocomposites. They consist in resin matrix reinforced with nanocrystalline Fe powders. Nanocrystalline Fe powders were obtained by high energy ball milling. The prepared samples at different milling times were characterized via X-Ray powder Diffraction (XRD) and Scanning Electron Microscopy (SEM).
Electromagnetic scattering parameters were measured within X-band metallic wave guide with rectangular section. Microwave conductivity and other electromagnetic parameters were deduced using the Nicolson-Ross-Weir (NRW) algorithm. Microwave conductivity and structural properties effects are investigated according to milling progression and frequency.

[1] R.C. Che, L.M. Peng, X.F. Duan, Q. Chen and X.L. Liang, Adv. Mater. 16, (2004).
[2] T. Galek, K. Porath, E. Burkel and U. Van Rienen, Modeling Simul. Mater. Sci. Eng.18 (2010)025015.
[3] Chen, L.F. Ong, C.K. Neo, C.P. Varadan, V.V. and Varadan, V.K. (2004). John Wiley & Sons Ltd, England.

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Structural Electromagnetic and Microwave Absorption Properties of Crni Based Nanocomposites

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In this work we investigate the structural, Electromagnetic and microwave absorption properties of CrNi based nanocomposites. Nanocrystalline CrNi powders were produced by high energy mechanical alloying route. Bulk nanocomposites samples are obtained by dispersing the nanocrystalline CrNi powders within resin matrix. The specimens are used to study their structural properties when subjecting to the action of an electromagnetic field and to measure the evolution of the reflection coefficient in the rectangular waveguide in an X-band instrument PM7001X, and characterized by several technics: SEM, EDX, XRD and DSC. Microwave dielectric permittivity, magnetic permeability and absorption spectra were determined using the Nicolson-Ross-Weir (NRW) algorithm. Their relationship to developed structural properties are discussed.

DSL251
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Optimization of High Energy Ball Milling Parameters of TiAlN Powder Synthesis

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Bulk materials based on supersaturated (Ti,Al)N solid solution fabricated by powder metallurgy approach are very attractive for a wide range of applications. In the present study the (Ti,Al)N nano-powder was synthesized by mechanical alloying using a planetary high energy ball milling (HEBM) Taguchi's method was applied to investigate the effect of main milling parameters: milling time (MT), ball to powder weight ratio (BPWR) and milling speed (MS) on the fraction of dissolved AlN in TiN during pure nitrides milling . The orthogonal experiments array was conducted and analyzed based on Taguchi's signal to noise ratio and variance techniques. The as-received and milled powders were characterized by X-ray diffraction (XRD). Analysis of variance (ANOVA) and main effect plot are used to determine the significant parameters and set their optimal levels. It was established that the milling speed is the most effective parameter on the fraction of the dissolved AlN. The optimum conditions for powder synthesis are: MS 600rpm, BPWR 50:1 and MT 50hours. The XRD analysis confirmed that homogeneous single phase nanostructured TiAlN powder is obtained under the optimized condition of HEBM.

DSL261
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Static and Dynamic Screening Effects in Diffusion-Controlled Self-Assembly of Charged Nanoparticles
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As is well known, nanoparticles (NPs) of different materials could be functionalized with charged ligands and used as building blocks in producing ordered structures in nanoscale self-assembly (SA) [1]. However, the fundamental problem of the interaction of the charged NPs embedded into the salt solution (polar solvent) remains unsolved. This is largely due to the fact that the outcome seems obvious: salt ions are expected to be redistributed around the NPs so that the long-range Coulomb potential becomes strongly screened and effectively transforms into a short-range (the static screening effects, a contribution associated with the rapid spatial redistribution of small and highly mobile ions of a solvent). However, this model has a limited range of applicability being valid only for infinitely diluted systems and high salt concentrations.

During a slow SA process very dense structural elements (aggregates) are formed, in which the distances between the NPs could become to be comparable to the Debye radius in the Yukawa potential [1]. For such the structural elements dynamic screening effects (the contribution of NPs themselves into the screening potential) becomes important. Using a novel integrated approach (nonlinear integro-differential kinetic equations for the correlation functions of particles), we have obtained the self-consistent solution in 3d case and compare roles of both static (quasi-equilibrium) and dynamic (non-equilibrium) charge screening effects in different situations [2,3].

[1] D. A. Walker, B. Kowalczyk, M. Olvera de la Cruz, and B. A. Grzybowski, Nanoscale, 3, 1316 (2011).
[1] V.N. Kuzovkov, G. Zvejnieks, and E.A. Kotomin, Phys. Chem. Chem. Phys., 16, 13974 (2014).
[2] V.N. Kuzovkov and E.A. Kotomin, Phys. Chem. Chem. Phys., 16, 25449 (2014).

DSL349
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Growth of Stress-Induced Ag Micro/Nanomaterials in Conductive Structure
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Ag micro/nanomaterials (MNMs) have vast applications in the fields of electronic devices [1] and transparent conductive electrode [2]. It is noted that electronic devices usually require conductive structure for assembly. Therefore, it is very attractive to fabricate Ag MNMs in conductive structure. Traditional approaches for forming Ag MNMs are based on chemical reactions. However, it is difficult to remove the impurities from the solution in which the reactions occurred, and these impurities affected the Ag MNM growth and their applications. On the other hand, it was reported that techniques based on stress migration (SM), which is a physical phenomenon, can be used to fabricate metallic MNMs [1]. To achieve metallic MNM growth by SM, a metallic film covered with a thin surface layer (e.g., natural oxide layer or artificial layer) are indispensable. The surface layer provides pathways for atomic discharge via weak spots. Thus far, Al, Cu and Ag nanowires have been fabricated on a Si wafer by using SM [3]. However, it is still a great challenge to obtain Ag MNMs with high yield in conductive structure by SM.

In this work, Al MNMs including nanowires and micro/nanoparticles were fabricated by using SM in conductive structure, and the effects of heating temperature and the thickness of surface layer on Ag MNM growth were also discussed. It was found that atomic flux in Ag film increased with increasing temperature.The stress gradient caused by mismatch of thermal expansion and material singularities provided the driving force, and the surface layer provided pathways for Ag atoms to discharge out.

[1] H. Tohmyoh, M. Yasuda, M. Saka, Scripta Mater. 63, 289 (2010).
[2] J. Lee, P. Lee, H. Lee, D. Lee, S. S. Lee and S. H. Ko, Nanoscale, 4. 6408 (2012).
[3] Y. Lu, H. Tohmyoh, M. Saka, Thin Solid Films, 520, 3448 (2012).

DSL356
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Biocompatible Hydrogel based Nanostructured Materials for Controlled Drug Delivery

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Polymeric materials with porous structure and high water contents are advantageous because of their tuneable mechanical and biochemical properties [1-3]. Synthetic or natural (bio)polymers are extensively explored for drug delivery and other medical applications. The amount and kinetic of the active agent release from the porous structure hydrogel can be adjust by the application of filler materials. Due to their lamellar structure, surface charge and biocompatible behaviours, clays and layer double hydroxides are widely used in biomedical applications [4,5]. The hydrophobization (functionalization) of initial lamellae with different surfactant molecules allows the immobilization of poorly water soluble molecules into the layers. Different drug molecules (Ibuprofen as painkiller and Mytomycin as chemotherapeutic agent) were encapsulated in layered structure inorganic drug carrier systems (negatively charged clay minerals and positively charged layered double hydroxide /LDH/). The synthetized composite were investigated by IR, XRD, SAXS and thermoanalytical methods. The active agent molecules were successfully intercalated into the interlayers. Next the prepared and characterised montmorillonite and LDH particles containing the drug molecules were encapsulated in pH and temperature sensitive biocompatible hydrogels for controlled drug release. According to the results the amount and kinetic of the released drug were highly adjustable by the synthesis conditions.

References
[1] L. Janovák, J. Varga, L. Kemény and I. Dékány. Colloid and Polymer Science, 286, 1575 (2008).
[2] L. Janovák, J. Varga, L. Kemény and I. Dékány. Applied Clay Science, 43, 260 (2009).
[3] L. Janovák, J. Varga, L. Kemény and I. Dékány: Journal of Thermal Analysis and Calorimetry, 98, 485 (2009).
[4] Á. Deák, L. Janovák, Sz. P. Tallósy, T. Bitó, D. Sebők, N. Buzás, I. Pálinkó, I Dékány: Langmuir, DOI: 10.1021/la504096t (2015)
[5] V. Hornok, T. Bujdosó, J. Toldi, K. Nagy, I. Demeter, C. Fazakas, I. Krizbai, L. Vécsei, I. Dékány: J Neural Transm., 119, 115 (2012).

VIP044
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Carbon Nanotubes Filled with Chalcohalides

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There is a great demand for control versatile electronic characteristics of CNTs. One strategy is to use the CNTs themselves, controlling useful properties via their radii and morphologies. CNTs are sp2 graphene carbon cylinders capable of hosting a variety of species, including 1D crystals of e.g. metals, metal salts, oxides, semiconductors and superconductors. Such objects are distinguished in their unique physical and chemical properties from both hollow nanotubes and the encapsulated substances, which permits one to purpose-tailor "nanowires" and "nanotubes" with unique physical and chemical properties. The presented very simple, sonochemical synthesis of nanophase chalcohalides in CNTs at low temperature is a convenient, fast, mild, efficient and environmentally friendly route for producing novel type of hybrid nanomaterials. It provides a "bottom−up" approach for the manufacture of future nanoscale devices. The ultrasonic nanowelding of this type nanodevices with metal microelectrodes meets the need of large-scale, simply, and efficient technology to build reliable interconnections between the CNTs filled with chalcohalides formed from the group 15–16–17 elements and the external electrical circuits. This paper summarizes results of investigations on electrical and photoelectrical properties of the carbon nanotubes filled with chalcohalides as gas sensors. Obviously, the new materials as the other one-dimensional semiconductor nanostructures should receive considerable attention from the scientific and engineering communities due to their potentially useful novel electronic properties.

Special Session 6
DRYING AND WETTING OF SOLIDS AND PARTICULATE MATERIALS (SS6)

DSL208
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A Flood Risk Criterion Applied to the Northern Portuguese Cultural Heritage

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The Portuguese building heritage is of great importance, justifying the need to safeguard it from extreme climatic phenomena such as floods and moisture degradation. For historical reasons the most prestigious buildings were built near the natural water lines and are possibly threatened by the flood phenomenon.

Climate changes due to global warming have revealed an increasing vulnerability of urban and rural territories to the risk of flooding. It is therefore necessary to adopt preventive measures to control, minimize and mitigate these adverse effects, avoiding catastrophic consequences.

This work presents a critical review of a criterion of risk, created to assess the flood risk of the Portuguese building heritage. In order to evaluate this criterion, it was applied to a sample of ninety monuments from the north of Portugal. In a first approach only two parameters were adopted: the shorter distance from the monument to the water lines and the height difference from the lowest point of the monument adjacent land to the plane of the closer water courses.

A final application exercise to a sample of northern Portuguese building heritage revealed a significant amount of monuments classified as medium or medium high risk of flood.

DSL217
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A Three-Dimensional Analytical Study of Water Absorption in Composite Materials Reinforced with Natural Fiber

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A major challenge in recent years is to develop new materials such as composites, to meet the growing worldwide demand for the use of these materials and reduce the impacts of its production, mainly environmental. Several researches have been conducted on the use of natural fibers as reinforcement in polymer matrix composites, due to the possibility of replacing synthetic fibers and their great potential for technological applications. However, water absorption affects the mechanical properties thereof strongly [1;2].

Thus, this study aims to theoretically study the behavior of water absorption in polyester matrix composites reinforced with plant fiber from pineapple leaf, with 20 and 40 % fiber content at environmental temperature. It was proposed a transient three-dimensional mathematical model to predict the mass transfer during water absorption

of these composites with rectangular shape. The exact solution of the governing equation has been done using the separation of variables. Predicted results of the moisture content distribution within the composites and its moisture absorption kinetic were provided and compared with experimental dates, in order to validate the methodology and estimate the mass diffusion coefficient. From this comparison was observed that increasing fiber content we have an increase in both water absorption and diffusion coefficient of the composite mass. The major moisture flux occurs in the vertex of the composites.

[1]L.U.Devi; S.S. Bhagawan and S. Thomas. J.Appl.Polym.Sci. 64, 1739-1748 (1997).
[2]A.K.Bledzki and J.Gassan. Progress in Polymer Science, 24, 221-274, (1999).

DSL286
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Wet Scavenging of Gaseous Atmospheric Radioactive Soluble Pollutants
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We analyze effects of inhomogeneous concentration and temperature distributions in the atmosphere, rain droplet evaporation and radioactive decay of soluble gases on the rate of trace gas scavenging by rain. We employ a one-dimensional model of precipitation scavenging of radioactive soluble gaseous pollutants that is valid for small gradients and non-uniform initial altitudinal distributions of temperature and concentration in the atmosphere. We assume that conditions of equilibrium evaporation of rain droplets are fulfilled. It is demonstrated that transient altitudinal distribution of concentration under the influence of rain is determined by the linear wave equation that describes propagation of a scavenging wave front [1]. The obtained equation is solved by the method of characteristics. Scavenging coefficients are calculated for wet removal of gaseous iodine-131 and tritiated water vapor (HTO) for the exponential initial distribution of trace gases concentration in the atmosphere and linear temperature distribution. Theoretical predictions of the dependence of the magnitude of the scavenging coefficient on rain intensity for tritiated water vapor are in good agreement with the atmospheric measurements of Piskunov [2]. The obtained results can be used in different meteorology-chemistry models, in particular in parameterizations of under-cloud scavenging of radioactive atmospheric soluble gases.

Keywords: Radioactive gases; Scavenging; Gas absorption; Atmosphere; Droplet evaporation; Precipitation

References
[1] T. Elperin, A. Fominykh, B. Krasovitov. Meteorology and Atmospheric Physics 125, 197 (2014).
[2] Piskunov, V.N., Golubev, A.V., Balashov, Y.S., Mavrin, S.V., et al. Atmospheric Environment 62, 573 (2012).

DSL299
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Drying Efficiencies under High Frequency Pulsed Fluidisation
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With a global concentration on emissions reduction, industrial efficiencies have become one of the most widely researched topics. Processes with a presence in multiple industries offer the greatest potential efficiency savings and are consequently at the forefront of development. One such process is that of drying, a key stage in fuels, food and chemical manufacturing. Of the numerous drying methods available, fluidised beds are one of the most common. Improvements to fluidised beds include the application of vibrations, acoustic fields, magnetic fields, mechanical agitations and pulsation of fluid flow. Research into pulsed flow or pulsofluidised beds as one of the more promising of these has to date found an improvement in heat and mass transfer rates[1], reduced slugging and channelling[2], improved fluidisation of hard to fluidise materials[3] and a reduction in product damage[4] and energy consumption[5], indicating a potentially significant efficiency improvement. However there are multiple methods of producing a pulsed flow, with corresponding differences in additional energy consumption, pulse frequency capacity and ease of manipulation to change the pulse frequency.

A novel approach to pulse generation is therefore suggested as an alternative, with the theoretical option of no additional energy requirements and variable pulse frequency. Drying efficiencies for a range of particle types are used as an indicator of the applicability of this approach. Whilst experimental research has typically been limited to a range of 1-15 Hz pulse frequencies [6], this research presents the results of applying a 270-320 Hz range of frequencies.

[1] A. Akhavan, et al., Ind. Eng. Chem. Res., 48, 302, (2009).
[2] M.-O. Coppens and J. van Ommen, Chem. Eng. J., 96, 117, (2003).
[3] S. S. Ali and M. Asif, Powder Technol., 225, 86, (2012).
[4] A. Reyes, et al., Dry. Technol., 30, 1368, (2012).
[5] M. Nitz and O. P. Taranto, J. Food Eng., 80, 249, (2007).
[6] D. Zhang and M. Koksal, Powder Technol., 168, 21, (2006).

VIP037
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Dehydration Controlled Applied to Viticulture

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Various studies have provided preliminary evidence about the influence of phenolics compounds, in the wine and grape juices, and the positive health effects. The partial dehydration the grapes, for winemaking or juices, shown be process to increased concentration of sugar and phenolic compounds in the must. The-chemical changes caused by harvesting activated metabolic processes and the stress caused by temperature difference induces the synthesis of phenolic compounds and aromatic substances, because the organic compounds are volatilized at certain temperature levels above the ambient temperature. These results justified the partial dehydration of grapes and the technological application, in low and high temperature, with control the thermal and psychometric parameters and monitoring of process, with benefits for the increased phenolic content and concentration of sugars and adequate ratio cost- benefit.

VIP055
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Osmotic Dehydration of Sweet Potato in Different Osmotic Agents: Experimental and Mathematical Aspects

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The sweet potato is a root from Latin America, eaten worldwide. Due to its low glycemic index carbohydrates, athletes nowadays consume it. The dried form could be a read to eat product and the osmotic dehydration (OD) is a pretreatment for drying. The aim of this work is to evaluate the experimental and modelled kinetics of OD of vegetables (sweet potatoes) in different osmotic agents (sucrose, fructose and sorbitol). Several diffusive models were tested to fit the kinetics. The results showed that diminishing water activity resulted higher water loss and solid gain, and that the solution with the highest water loss was the sucrose, followed by sorbitol and fructose in all conditions. The highest solid gain was obtained by using fructose, followed by sorbitol and sucrose.

DSL205
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Numerical Study of Particle Deposition during Droplet Evaporation on a Solid Surface

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Droplet evaporation and particle deposition on a solid surface has attracted increasing attention as an efficient fabrication process for display and micro devices [1,2]. However, its general predictive model has not yet been developed due to the complexity of the multiphase phenomena.

Recently, numerical simulations of the process has been performed using a finite-element method (FEM) [3,4] and a body-fitted moving-grid method [5] to solve a diffusion equation for the vapor fraction and an advection-diffusion equation for the particle concentration. However, the Lagrangian methods are generally not straightforward to implement for breaking or merging of the interface.

In this study, a sharp-interface level-set method, which can easily handle the liquid-gas interface with change in topology, is developed for comprehensive simulation of droplet evaporation and particle deposition including the effects of evaporation, mass transfer, heat transfer, and dynamic contact angles. The numerical simulation of particle distribution in droplet evaporation demonstrated the particle accumulation (or coffee-ring formation) near the liquid-gas-solid contact line. The effects of contact angle and particle diffusion on the droplet evaporation and particle distribution are quantified.

[1] R.D. Deegan, O. Bakajin, T.F. Dupont, G. Huber, S.R. Nagel and T.A. Witten, Nature, 389, 827 (1997).
[2] A. F. Routh, , Rep. Prog. Phys., 76, 046603 (2013).
[3] E. Widjaja and M.T. Harris, AICHE J., 54, 2250 (2008).
[4] R. Bhardwaj, X. Fang, and D. Attinger, New J. Phys., 11, 075020 (2009).
[5] K. L. Maki and S. Kumar, Langmuir, 27, 11347 (2011).

DSL207
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Experimental Tests on a Dryer Solar of Exposure Indirectly Used to Produce Dried Bananas

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This paper presents the results obtained in the process of drying bananas using solar energy, in order to spread the culture of renewable energy and to promote sustainable development. The use of solar energy is important because of its characteristics of being clean and widely available throughout Brazil, mainly in the Northeastern part of Brazil. Developing equipments using solar energy as an energy source in the Northeastern region of Brazil contributes to promote social-economic growth, thereby reducing social inequalities in the region [1]. Among the various types of fruits produced in Brazil, we chose bananas because of its large domestic production, and its economic and nutrition contribution. Bananas have great postharvest losses, since it is extremely perishable. The study aims to change fresh bananas in dried bananas, which has high added value. The solar drying of banana with the use of indirect radiation dryers turns to be a viable alternative to small, medium and large bananas producers [2]. We present data obtained from experiments on drying bananas through the solar dryer developed in UFCG. The experiments showed statistical significance, and the used empirical model proved to be reliable and representative because of the high values of the correlation coefficients that approached 0.99. In this work, we also present the constructive and operational characteristics of the equipment under development.

[1] M.B. Grilo, A.P.F. Leite, R.R.D. Andrade and F.A. Meunier, Renewable Energy, 32, 697, (2007).
[2] A. G. Nunes, I.A. Gomes and M.B. Grilo, Magistra, 26, 1749, (2014).

DSL221
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Applying Liquid Diffusion Model for Continuous Drying of Rough Rice in Fixed Bed

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Simulate the rice drying process at specific drying conditions is of great interest to optimize the process and ensure a better quality of the final product. Several mathematical models have been used to describe the mass transport during drying of rough rice grains [1, 2]. In the present work, experimental drying procedures of rough rice grains long-thin (BRSMG CONAI variety) was reported and drying kinetic were obtained at temperature of 40°C. The results were compared with simulated data by means of the liquid diffusion model with equilibrium boundary condition. The geometry used to represent the rice grain was prolate spheroid. For this purpose, the diffusion equation, written in cylindrical coordinates, was resolved via Galerkin-based integral method considering the constant diffusion coefficient. A good agreement was observed between modelling and experimental data. The inexistence of constant drying rate period was verified, proving that diffusion is the main mechanism responsible for the moisture loss. It was also possible to observe that the highest moisture gradients occur at the tip of the grain, which is region more affected by thermal and hydrics stresses. The proposed model can be used to solve

problems involving diffusion processes, such as: drying, wetting, heating and cooling, provided that the geometrical shape of the body is similar to prolate spheroid.

[1] A. Cihan, K. Kahveci and O. Hacihafızo lu, J. Food Eng, 79, 293 (2007).
[2] O. Hacihafızo lu, A. Cihan and K. Kahveci, Food and Bioproducts Processing, 86, 268 (2008).

DSL227
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Drying of Rough Rice Grain (BRSMG CONAI Variety) in oven at Temperatures of 60 and 80oC

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Rice (Oryza sativa L.) is a crop of great socio-economic importance, mostly because it is the basic component of the diet of most of the world population, source of energy, protein, vitamins and minerals [1]. For the individual farmer, immediate threshing and drying of wet harvested grain to 18–19% (w.b) moisture content is a practical method to arrest deterioration and increase selling price. The grain of rough rice is different from other grains because it has a cover outer shell (palea and lemma) and a layer of bran. Therefore, the heat and mass transfer processes occurring in paddy grain drying are different from other cereal grains. Harvest season and drying of the grain are the most important factors that influence the characteristics of rice seed, to be sown or consumption. Therefore, understanding the effect of various treatments and drying temperature and content moisture gradients occurring in the fissure grain of rice is essential to optimize the drying conditions [2]. This study aimed to analyze the behavior of removing moisture in oven at temperatures of 60 and 80oC, stress cracking and yield of the number of grains of rice whole. The experimental data were subjected to individual analysis of each temperature. It is concluded that reducing the water content of the grains is considered to be very complex and may substantially alter its physical properties and quality of the product, depending on the method and conditions of drying.

[1], M. Walter, M. Marchezan and L. A. Avila. R. Sci, Santa Maria., Vol. 38, n.4, p.1184 (2008).
[2] R. Dong, Z. Lu, Z. Liu, S. Koide and W. J. CAO, J. Food Eng., Vol. 97, n.1, p.167 (2009).

DSL228
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A Theoretical Investigation of Banana Drying using Diffusion Model

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Fresh fruits are dried after harvesting, in order to reduce the waste and the spoilage and to extend their shelf life. Overall post-harvest losses of fruit and vegetables in developing countries are estimated at about 20–50% of the production. During the drying of fruits and vegetables occurs big variations of the volume and surface area of the product simultaneously with the loss of moisture and increase of the temperature. From the viewpoint of consumption, bananas are fruits with aromatic flavor which are naturally sweet. They provide flavor and variety to the human diet, and also serve as an important source of essential vitamins and minerals, although they are not good and economical sources of protein, fat and energy. They contain different constituents such as fat, high natural sugars content, protein, potassium and vitamins A, B complex and C. Due to the sequential growth of banana cultures and the amount of harvested banana, losses of these fruits has increased and thus generates the necessity of studies for conservation of these fruits [1-2].

This work presents a theoretical drying study of banana fruit using diffusion model (Fick´s law). The governing equation was solved by using the separation of variables technique. For validation, whole banana were peeled manually and dried in an oven at temperatures 40 and 70oC. Predicted results were obtained and fitted to experimental data using the least square error technique. Results revealed which air temperature affect significantly drying of banana. The fitted results presented good concordance with the experimental data.

[1] A. M. D. Karim and M. N. A. Hawlader. J. Food Eng. 70, 35-45, (2005)
[2] V. C. Mariani; A. G. B. Lima and L. S. Coelho. J. Food Eng. 85, 569-579 (2008).

DSL231
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Transition from Superhydrophobic to Superhydrophilic Surface with Random Nanorod Arrays

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Micro/nano structured surface presents extreme water-repel behavior by the entrapment of air bubbles in the grooves beneath the water (called Cassie state). However, this ultra hydrophobicity can be invaded through the impalement of water into the grooves (Wenzel state), to say, the Cassie–Wenzel (C-W) transition happens. This transition can be triggered by the evaporation of water drop, which arise the question how to maintain the superhydrophobicity to make the surface dry.

Recently, some sophisticated micro pillars have been designed to understand the mechanism of the C-W transition, where, a critical Laplace pressure Pc was determined by the geometric parameters on the surface texture. However, irregular pattern with random dimension of the texture asks the question how to define this transition. Here, we design an intriguing nanostructure of ZnO nanorod array, with the diameter of 190 nm and randomly growing on the flat substrate. Surprisingly, we find a much larger contact radius (~250 µm) for the starting of the C-W transition, which is unpractical from the prediction based on the periodic micro-structured. Additionally, three regimes of the evolution of the contact angle are proposed for the lifetime of the drop evaporation on the ZnO nano-structured surface. Accordingly, we propose that the C-W transition starts much early due to random surface geometry, and the amount of the Wenzel state accumulates and finally contribute the rapid dropping of the apparent contact angle. Therefore, here a trigger and critical of C-W transitions are newly defined separately. In addition, we introduce the deposit formation during the evaporation, which enhances the pinning effect. The coupling of the pinning and evaporation makes the complex of the pattern and morphology of the dry deposit, which allows us to control the macro capsules preparation by using the evaporative drop with colloidal suspension in present work.

DSL232
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Mechanical Characterization and Water Sorption in Polyester Matrix Composites Reinforced with Sisal Fiber: An Experimental Investigation

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The use of vegetable fibers as reinforcement in polymer composites with the aim to replace totally or partially synthetic fibers has received much attention in recent years. This is due to the fact that the vegetable fibers presented good advantages such as: low density, good strength, is non-polluting, and are originating from renewable sources [1]. However among the main disadvantages of natural fibers is their high moisture absorption which reduces their adhesion with the matrix causing failures. The failure in composites should occur in the matrix, but as adherence is never perfect, the process of rupture is generated at the interface. Therefore, in most cases, the failure of the reinforced polymer occurs by shear in the interfacial region [2].

In this work we evaluated the mechanical characterization of polymer matrix composites reinforced with sisal fibers in the dry and saturated conditions and the water sorption as a function of time and temperature. Experimental tests of tensile (ASTM D 3039), impact (ASTM D 256) and water sorption in samples with rectangular cross section were made. The polymer matrix used was the unsaturated polyester resin (Resapol 10-316). With the aim of analyzing the mechanical properties of the composite as a function of the fiber content, samples were manufactured with different amounts of fiber (mass/mass): 20 and 44.6%. For the water sorption test was selected the composite with fiber content which showed the best results in the mechanical tests. In the experiments, the specimens (tensile, impact and sorption) with fiber content of 44.6% were immersed in water at ambient temperature until to achieve equilibrium condition (saturation point). After reaching the equilibrium, the composite moisture content curves were made as a function of time and temperature. Saturated samples were also subjected to tensile and impact tests to analyze the decrease in property values due to moisture content.

Keywords: sisal fiber, unsaturated polyester, mechanical properties and water sorption.

[1] A. K. Bledzki and J. Gassan, Prog. Polym. Sci., 24, 221 (1999).
[2] M. M. S. Nobrega. Polyester matrix composites with caroá fibers (Neoglaziovia variegata): mechanical characterization and sorption of water. Doctorate Thesis, Process Engineering, (Federal University of Campina Grande, Campina Grande, Brazil, 2007).

DSL236
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Microwave drying of Prolate Spheroidal Solids via Finite Volume Method

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Drying is the process of removing moisture in the product up to certain threshold value. The effectiveness in drying techniques can be evaluated on two levels: cost of the process and final product quality. In some cases, the drying time becomes important in view of production speed. In the case of food product quality: appearance and biological value are irrelevant to the drying time [1]. Microwave drying offers to shorten the drying time without degradation of final quality of the dried product. This work aims to develop a mathematical model and numerical study of heat and mass transfer in prolate spheroidal solid via finite volume when exposed to microwave. The model considers boundary condition of the third kind and variables thermophysical properties. A numerical code based in [2] has been implemented for evaluation of solid moisture content and temperature at different instants of drying process. The mathematical model predicts that the moisture content is reduced more quickly at the tip of the solids, thus this region is most favorable to fracture and warping of the product due to high moisture and temperature gradients. Moreover, it is observed that the temperature decreases from the surface to the center of the solid and increased drying time.

[1] I. Hammouda and D. Mihoubi, Energy Convers. Manage., 87, 832 (2014).

[2] V. A. B. Oliveira. Heat and Mass Transfer inside of Solids with Prolate Spheroidal Shape Via Thermodynamics of Irreversible Processes. Doctorate Thesis, Process Engineering, Federal University of Campina Grande, Campina Grande, Brazil, 2006.

DSL239

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An Experimental Study on the Drying Kinetics of Castor Bean Fruits (Ricinus communis L., "Br Energia" variety)

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Castor bean is considered to be native to tropical Africa, but is cultivated in many tropical and subtropical regions of the world [1]. The India is the world largest producer of Castor oil seed with annual production of 1.64 million tons, followed of the China, Mainland China, Mozambique and Ethiopia with productions of approximately 60, 60, 60 and 13 mil tons, respectively [2]. Castor bean is an oilseed relevant economic importance to Brazil, being traditionally produced on small and medium farms, generating jobs and income due to its numerous application possibilities in industry area [3]. The castor bean consists of approximately 50% oil. This oil has special characteristics such as high viscosity, heat and pressure stability, low freezing point, and the ability to form waxy substances after chemical treatments [4]. Therefore, the castor bean is a potential candidate for the production of biodiesel. However, this product must be dried, in order, to reduce moisture content, for safe storage. This work aims to conduct an experimental study of the drying kinetics of castor bean fruits (Ricinus communis L., "BRS Energia" variety). Experiments were conducted using oven on the air temperatures 50 and 70°C and relative humidity values 16.34 and 6.24%, respectively. The experimental moisture content data as function of time were fitted to some models (namely Henderson and Pabis, Page, Midilli and two-term exponential models) available in the literature, and a good agreement was observed. The values of the effective moisture diffusivity, Deff were obtained from the Fick's diffusion model. The value of activation energy (Ea) was determined assuming the Arrhenius-type temperature relationship.

[1] G. Allan, A. Williams, P. D. Rabinowicz, A. P. Chan, J. Ravel, P. Keim, Genet Resour Crop Ev, 55, 365 (2008).

[2] FAO, Food and Agriculture Organization of United Nations: Information on: www.fao.org. Access in: December 2014.
[3] A. L. D. Goneli, P. C. Corrêa, F. E. A. Magalhães and F. M. Baptestini: Acta Sci., Agron. (Online). Vol. 33, n. 1, (2011), p.1-8. (In Portuguese)
[4] M. M. Conceicão, R. A. Candeia, H. J. Dantas, L. E. B. Soledade, V. J. Fernandes, A. G. Souza, Energy Fuel, 19, 2185 (2005).
[4] M. Chandrasekaran, Valorization of Food Processing By-Products, p. 836, Ed. CRC Press, Boca Raton, 2012.

DSL244
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Composites Reinforced with Vegetable Fiber via RTM (Resin Transfer Molding): Mechanical Characterization

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A composite material is made by combining two or more materials to give a unique combination of properties. The composites reinforced with vegetable fibers have important advantages: Low cost, low density, stregth, low abrasiveness to prossesing equipment, are biodegradable, are not toxico or polluting [1]. There are a wide variety of processing methods available to produce polymer matrix composites, which can be classified into an open mold processes (guide molding, spray), closed mold processes (injection molding, compression molding, resin transfer molding) and continuous processes (pultrusion, production of laminates). The RTM process for manufacturing polymer composites that is increasingly used especially for the automotive, maritime and aerospace sectors, and consists of injecting a polymer resin through a fibrous reinforcement pre-placed within the mold [2]. Resin Transfer Molding (RTM) consists of a low environmental impact process, because the processing is performed in a closed system, controlling the undesired emissions. There are some variations of the traditional RTM process such as RTM and VARTM Light.

This work aims to evaluate the mechanical characterization of polymer matrix composites reinforced with vegetable fibers via RTM. Experimental tests of tensile (ASTM D 3039), impact (ASTM D 256) in samples with rectangular cross section were made. The polymer matrix used is the unsaturated polyester resin. The analysis of the mechanical properties was performed according to the number of layers.

[1] A.K. Bledzki, J. Gassan. Prog. Polym. Sci., 24, 221 (1999).
[2] R. Gerlach, C. R. Sivion, N. Petrinic, J. Wiegand, Polym., 49, 2728 (2008).

DSL282
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Energetic and Exergetic Analysis of the Clay Bricks Drying in an Industrial Tunnel Dryer

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For centuries energy saving has been a basic requirement for economic development of the countries in the world, as a result of the growing energy consumption for the population and industries. Drying is a simultaneous process of heat and mass transfer including dimension variations requiring intensive-energy consumption. During the drying of ceramics products, heat is transported to the liquid inside the solid and simultaneously moisture is transported to out of solid. These phenomena provoke stresses. Depending on the drying conditions, structures of the material and geometry of the product, this phenomenon can cause cranks, deformations and even fracture inside the solid [1,2,3], which reduces product quality.

In this sense, the purpose of this paper is to present a theoretical study of industrial hollow bricks drying in a tunnel dryer cross flow type. The theoretical model is based on the 1st and 2nd laws of Thermodynamic applied to to the system. To validate the methodology, numerical and experimental results for the moisture content and the temperature of brick during the drying in an industrial scale are compared and a good correlation was obtained. Results of moisture content and temperature of the product and air, and energy and exergy efficiency are presented and analyzed.

[1] W.D. Callister, Jr. and D.G. Rethwisch: Fundamentals of Materials Science and Engineering: An Integrated Approach (3rd. ed. John Wiley & Sons, Inc. USA, 2008).
[2] J.F.M. Velthuis, Simulation model for industrial dryers: reduction of drying times of ceramics & saving energy, in: Proceedings of the International Drying Symposium (Drying' 96), Krakow, Poland, 1996, pp. 1323-1328.
[3] G. S. Almeida, J. B. Silva, C. J. Silva, R. Swarnakar, G. A. Neves, A. G. B. Lima: Applied Thermal Eng. 55, 78-86 (2013).

VIP012
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On the Use of Spheroidal Coordinates to Modeling of Wet Porous Ellipsoidal Solids in Drying Process

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Drying is an oldest method applied to moisture removal in wet porous solids. This topic is an important subject to be discussed not just amongst chemical and mechanical engineers but mathematicians and physicists as well. This technique usually requires very expensive equipment and high energy consumption, especially in situation where high temperature are used. Thus, several mathematical models have been proposed to accurately describe drying process. They are based on the conservation laws of heat and mass transfer or simply empirical equations based in drying experiments. Most of these models are based on the assumption of spherical or cylindrical solids. In many situations the shape of the porous solid is not perfectly spherical or cylindrical. Accurate modeling of the process of moisture removal in solids with complex geometry is only possible with accurate description of the geometry of the solid.

In this lecture, the transient diffusion equation written in spheroidal coordinates is presented [1-2]. The resulting unsteady diffusion equations are solved by using both the numerical (finite-volume) and analytical (separation of variables) methods describing heat and mass transfer for oblate and prolate spheroidal solids, considering constant or variable diffusion coefficient.

This work briefly focuses some of different models used today, including applications (wheat and lentil grains drying), elucidating the main physical aspects and limitations of these models. Further, the importance of the simulation as tools in the development, design and analysis of drying systems is discussed too.

[1] J. E. F. do Carmo, A. G. B. de Lima, Drying Technol., 23, p. 1977 (2005).
[2] A.G.B. Lima, S. R. Farias Neto, W. P. Silva, Heat and Mass Transfer in Porous Media, Vol.13, p.161, J.M.P.Q. Delgado, Ed. (Springer-Verlag, Heildelberg, 2012).

VIP030
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Water Sorption of Vegetable Fiber Reinforced Polymer Composites

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Despite the ever-growing worldwide interest in the use of lignocellulosic fibers as reinforcement in either thermoset or thermoplastic matrices, the use of these fibers to replace synthetic ones is limited. The reasons for this limitation is mainly associated with the vegetable fiber´s heterogeneity, lower compatibility to polymers, inferior durability, flammability, poorer mechanical properties and higher moisture absorption when compared with synthetic fibers. Nevertheless, despite these drawbacks, vegetable fiber reinforced polymer composites are lighter in weight, more sustainable and can be used for non-structural products. Strategies to minimize these drawbacks include fiber and or matrix modification, the use of compatibilizers, fiber drying and the concomitant use of vegetable and synthetic fibers, for the production of hybrid composites, the latter being an unquestionable way to increment overall mechanical and thermal properties of these hybrid systems. Here we present data on the water sorption of thermoset and thermoplastic matrices polymer composites as a function of vegetable fiber identity, content and hybridization with glass fibers. Our data indicates that, regardless if the matrix is a thermoset or a thermoplastic, water absorption tends to be relatively independent of vegetable fiber identity and to be significantly dependent of its content. Hybridization with glass fibers leads to lower overall water absorption and higher mechanical properties.

DSL334
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Role of Electrical Field in the Diffusion Regime on Osmotic Dehydration of Apples

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The diffusion in biological tissue does not necessary fulfill the conditions to observe Fickian diffusion. Specifically, the diffusion of sugars in apple tissue during osmotic dehydratation has been shown that present a non-Fickian diffusion. This anomalous diffusion correspond to a super diffusive case which was modeled using fractional calculus.

The coupled application of an electrical field has been used in osmotic dehydration to improve process in term of time and final water content. The Granny Smith Apple variety was used as a substrate. The osmotic solution was prepared using sucrose in the range 45-65 ° Brix. The electrical field applied ranges from 0 to 17 V/cm.

It was observed that for moderate electrical field the diffusion regime transition from a super-diffusive scheme a Fickian diffusion. This could be explained by effect of the electrical field in the food microstructure, corresponding to electroporation. This not also increase the mass transfer rate, also affects the diffusion paths, avoiding channelling thus given the conditions to observe Fickian diffusion.

Special Session 7
HEAT AND MASS TRANSFER IN POROUS MEDIA (SS7)

DSL091
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Numerical and Experimental Study of Water Flow in Ceramic Membranes used in Microfiltration

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Over the past two decades, membrane filtration processes have played a more and more important role in industrial separation process. Many studies have focused on the best ways of using a particular membrane process. Computational fluid dynamics techniques may provide a lot of interesting information for the development of membrane processes. Numerous improvements of the technology have allowed membrane selection for a particular process to be done more easily and more quickly.

In this sense, in this paper we present a numerical study of the process of separation by ceramic membranes. We adopted a system in which only water flows through the membrane to obtain a mathematical model able to predict the behavior of water permeation in the membrane observed experimentally. The value was considered constant porosity and permeability of the ceramic membrane as a function of the resistance to flow of the porous medium. The numerical study considering a three-dimensional computational domain was performed using the commercial package ANSYS CFX 12 using the full equations of momentum and continuity equation. We adopted the model of turbulence RNG k-e. We evaluated the results of pressure and velocity fields. It was also performed a comparison of numerical data transmembrane flux with the experimental data.

The numerical results showed that the mathematical model used can fit to the experimental data, the increased resistance of the porous due to hydration was found to be greater than 1000%, the pressure and velocity profiles are presented and analyzed.

DSL258
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Heat Transfer Analysis of Evaporating Meniscus in High Aspect Ratio Microchannel

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Evaporating meniscus of ethanol in single flat microchannel was experimentally investigated. An integrated testing system including syringe pump, microchannel test section, high speed camera and infrared camera was mounted in a 1 m3 plexiglass box, the ambient temperature inside of which was controllable. Different microchannels were tested, the hydraulic diameters of which are 571, 727 and 1454, and the cross sectional aspect ratio is 20, 20, and

10 respectively. The channel was vertically positioned. During the experiment, a meniscus was maintained in the channel at a constant altitude by ajusting the heat flux and syringe pump flow rate. Visualisation and thermographic results of the stationary meniscus at various evaporation rates were obtained.

The dependencies of the meniscus evaporation rate and the specific evaporation rate on heat flux in different microchannels were studied to examine the dominances of channel cross sectional geometry and the length of the contact line during evaporation. Besides, the temperature profiles along the meniscus were extracted from the thermographic measurements. Furthermore, a simplified theoretical model was presented for the calculation of evaporation rate in high aspect ratio microchannel, considering the heat conduction within the microchannel wall and the heat stored in the superheated layer near the channel inner surface. Comparisons between the calculations with the experimental results were made. The influence of the channel cross section corners on the evaporation heat transfer process was highlighted.

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Modeling and Simulation of Dispersed Surfactant Injection in Gas-Condensate Reservoirs: A Phenomenological Approach

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Recent developments in gas phase stimulation techniques (GaStim) [SPE 152309, SPE 168133] indicate that the gas phase as carrier fluid enables a better transport and mobilization of the chemical agent in the reservoir. In this work we model the transport of a surfactant carried by a compressible fluid in a reservoir with gas-condensate blockage and it is represented through multiphase/multicomponent reservoir simulator. The understanding of underlying physical & chemical phenomena of surfactant flooding in the reservoir plays an important role in the effectiveness of a well stimulation procedure. For a given reservoir fluids-matrix-surfactant system, a limiting surfactant concentration may determine the technical/economic success or failure of the well intervention.

Therefore, an accurate modeling and simulation of the coupled transport and retention mechanism are important for the surfactant deployment design. Some processes are: surfactant advective, diffusive and dispersive transport, mixing and dissolution of surfactant with miscible phases, micro-emulsions generation, surfactant adsorption on matrix surface, surface and interfacial forces alteration, and others. The model considers the surfactant dissolution in the water and oil phases and the further adsorption on the matrix surface. The flow model equations are based on Darcy-scale macroscopic mass balance equation. The surfactant transport equation considers the advective, molecular and diffusive transport mechanisms and the mass transfer with miscible phases and matrix adsorption as well.

Flow and transport equations are solved following the finite-volume method with a second-order discretization scheme. The model predicts the evolution of surfactant distribution in the reservoir in matrix and soluble phases. The oil recovery factor can be estimated for a given well intervention. The model can be used for deployment optimization procedures in GaStim projects.

Keywords: Modeling, Simulation, dispersed surfactant, multiphase flow, adsorption.

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Single-Well Modeling and Simulation of In-Situ foam Generation for Gas Inyectivity Control
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Foams are being used in enhanced recovery operations as mobility control agents because they reduce the mobility of gas through preferential channels, while improving sweep efficiency of un-swept zones. Therefore, an incremental oil recovery is expected with the use of foams. A correct understanding of transport, generation and stability mechanisms is mandatory for the conformance design in order to generate a stable foam with an appropriate texture to guarantee the success of the procedure.
Transport and stability of foams is dependent on the type of foaming agent, its concentration and interaction with reservoir fluids, adsorption and desorption on the rock, pressure and reservoir temperature, surface tension between fluids and capillary pressures and other complex factors. Surfactants reduce gas mobility by stabilizing the liquid lamellae that cause the gas remains as a discontinuous phase. Generation mechanisms include snap-off, leave behind and lamellae division. Destruction mechanisms include condensation and evaporation, coalescence by the presence of oil.

In this work we model and simulate the generation and transport of foams in heterogeneous reservoirs, using a population balance model of trapped and mobile foams. Foam model is coupled to the transport model and adsorption of the foaming agent as well as the multiphase flow model. The numerical solution is based on the finite-volume method, using a second-order discretization scheme. Numerical experiments showed that the sweep efficiency increases in c.a. 10% when conformance is done with in-situ generated foams.

Keywords: Foams, Generation-Destruction, Models, Adsorption, Desorption, transport, recovery factor.

DSL301
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Numerical Modeling of Convective Drying of an Apple Slice
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Convective drying is widely used to dry porous materials ranging from brick, wood and paper, to grains, vegetables and fruit, to name a few. Numerical modeling is extremely useful as a design tool for simulating such problems. While various numerical approaches have been developed over the past decades, a recent approach developed by Khan et al. [1] simulates simultaneous heat and moisture transfer in conjugate fluid/porous domains, and can be used to simulate convective drying of porous materials. The key advantage of this formulation is that heat and mass transfers inside the porous region and at interfaces between porous and pure fluid regions is accounted for in a true non-equilibrium framework. In the present study, convective drying of an apple slice is considered, wherein the apple slice is considered to be a porous material comprised of solid and void. The void space is characterized by a porosity and assumed to be filled with an air-water vapor mixture. The solid constituent in the porous region is considered to be comprised of "flesh" (solid matter) and liquid water. Proper modeling of the apple slice as porous material requires thermosphysical properties of both the fluid and solid-constituents, and coefficients to characterize the transfers between phases. However, a literature survey reveals an absence of some key properties that require determination. In this respect, the major unknown is the moisture diffusivity coefficient of the fluid and solid-constituents of the porous region. These coefficients are determined herein by a

convective drying simulation that utilizes the effective moisture diffusivity determined by Velić et al. [2] in a highly-referenced experimental study on apple drying. The evaluated coefficients along with the necessary properties are then utilized to simulate the convective drying of an apple slice in a 3D domain as described in Velić et al. [2]. The present simulations show excellent agreement with the experimental data of Velić et al. [2] and provide detail that has not been presented in any prior simulations of convective drying.

[1] F.A. Khan, C. Fischer, and A.G. Straatman, Int. J. Heat Mass Tran., 80, 513 (2015).
[2] D. Velić, M. Planinić, S. Tomas, and M. Bilić, J. Food Eng., 64, 97 (2004).

DSL350
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Surface Tension Effects on a Conjugate Laminar Film Condensation Process on a Vertical Fin Immersed in a Porous Medium

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In this work we treat theoretically the film-wise condensation on a vertical fin embedded in a homogeneous porous medium. In this work we consider a two-phase region between the liquid film and the vapor region, where both condensate and vapor are present. When both liquid and vapor phases co-exist in the presence of solid surfaces, it is natural to consider the effect of surface tension [1, 2, 3]. In order to predict the influence of surface tension and the conjugate heat transfer on the thickness of the condensate, due to the porous medium, an overall energy balance in the liquid and the two phase zones was conducted. Additionally, the conservation equations of mass, momentum and energy on the liquid, and the energy equation in the fin are reduced to a nonlinear system of two differential equations with five dimensionless parameters: the Bond number, Bo, Jakob number, Ja, Rayleigh number Ra, a conjugate heat transfer parameter which it represents the competition between the heat conducted by the fin in the longitudinal direction with heat conducted through the condensate film, and the aspect ratio of the fin. Using the limits of Ja<<1, Bo<1, Ra=O(1), we applied perturbation methods and the boundary layer approximation to obtain the nondimensional heat transfer given by the Nusselt number, Nu, the fin efficiency and the mass flow rate of the condensed fluid as functions of the involved nondimensional parameters.

[1] K. S. Udell, ASME Journal of Heat Transfer, 105, 485 (1983).
[2] A. Majumdar and C. L. Tien, ASME Journal of Heat Transfer, 112, 751 (1990).
[3] M. Kaviany, Principles of Heat Transfer in Porous Media, p.605, Ed. (Springer, USA, 1999).

DSL229
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Drying Analytical Study of Hollow Ceramic Materials using Galerkin Based Integral Method

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One important stage in several productive processes, in the most different areas of human activity, is that regarding the drying of bodies or products constituted by porous materials. For instance, drying is used in the following fields: foodstuff, pharmaceutical, ceramics and paper industries [1]. The drying is the phase of the process that precedes firing and needs an appreciable amount of thermal energy to evaporate the water which was added during the molding process [2]. For more precise process of drying, it is important to consider the form factor of the body in the development of the mathematical model in order to describe the physical phenomenon, of more real way, and raise the confidence level of the model. Thus, the aim of this work is to develop an analytical solution for the transient mass diffusion equation in hollow ceramic products with arbitrary shape by using Galerkin based integral method (GBI method), by considering constant thermo-physical properties and equilibrium boundary condition at the surface (Dirichlet condition). Several results of the drying kinetics and moisture content distribution inside the solids are presented, analyzed and discussed.

[1] W.P. Silva, V.S.O. Farias, G.A. Neves, A.G.B. Lima, Springer-Verlag, 2011.
[2] W.D. Callister Jr., D.G. Rethwisch, An Integrated Approach, 3rd. ed., John Wiley & Sons, Inc, USA, 2008.

DSL234
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Inverse Engineering of Micro-Pore Tortuosity in Clays Via Pore Network Models
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Tortuosity of pore space influences the transport of water, solutes, and gases in porous media. For many applications, the desired pore network structure can be dictated in terms of tortuosity. This study proposes a method to inverse-engineer micro-tortuosity based on a microstructure-informed meso-scale pore network model. The model is intended for media where the pore geometry data acquired experimentally represents a fraction of total porosity. The chosen medium is Opalinus clay in the work. The micro-tortuosity in Opalinus clay is obtained by simulating diffusion of solutes with different molecular sizes. The analyses suggest that a major diffusion-controlling factor is the turtuosity of the micro-pores, i.e. the pores less than 5 nm. Further model improvements require better knowledge of their turtuosity, which awaits higher resolution experimental techniques. One way to verify assumptions for micro-pore tortuosity in such models is to conduct diffusion experiments of solutes with several different molecular sizes. Results for diffusion of three different species are presented to demonstrate the clear separation of diffusivity ranges, allowing for effective programme for inverse-engineering.

DSL254
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Multicomponent Gas Diffusion in Non-Uniform Tubes
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In many technical processes gas multicomponent diffusion takes place in confinements that are rarely uniform in direction of their long axis (e.g., catalysts pores, microelectromechanical systems). Here, we show that in conical tubes multicomponent diffusion is significantly hindered. This effect increases with ratio of inlet to outlet cone radius Λ, indifferent of the orientation of the tube. Based on the Maxwell–Stefan equations, predictive analytical solution for ideal multicomponent diffusion in slightly tapered ducts is developed. In two-bulb diffusion experiments on a uniform tube, the results of Duncan and Toor [1] were reproduced. Comparison of model and experiment shows that the solution presented here provides a reliable quantitative prediction of the temporal change of H2, N2, and CO2-concentration for both tube geometries, uniform and slightly conical. In the demonstrated case (Λ = 3.16), mass diffusion is 68 % delayed. Thus, for gaseous diffusion in "real," typically tapered pores and systems the transport limitation is more serious than considered so far.

[1] J.B. Duncan and H.L. Toor, AIChE Journal, 8, 38-41 (1962).

DSL327
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A Comparative Experimental Study on the Deviation of the Ideal Selectivity in HDTMS-Functionalized and untreated Ceramic Structures with Pores in the Upper Mesoporous Range
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In microfluidic systems, biotechnology and separation science, surface modifications of inorganic substrates are an active field of research. Mesoporous ceramic capillary membranes with mean pore sizes of about 20 nm are prepared as model structures to investigate the influence of an altered surface chemistry on the flow behavior of gases. To modify the membrane surface, a wet chemical silanization process with hexadecyltrimethoxisilane (HDTMS) is used to gain an alkyl-functionalized surface. Structural and surface characterizations show that the surface chemistry is altered without affecting the mean pore diameter. For the non-functionalized membrane, single gas permeation measurements reveal ideal permselectivities which are in good agreement with the Knudsen theory. After HDTMS-functionalization, the permselectivities regarding carbon dioxide deviate about 20 % from the aforementioned theoretical expectations, indicating a relative flow enhancement for carbon dioxide. Adsorption and desorption measurements show a decreased specific adsorption capacity, indicating a weaker interaction of gas molecules and surface due to HDTMS functionalization. This weaker gas-solid interaction is proposed as reason for the experimentally observed deviation of the permselectivities from Knudsen theory.

DSL371
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Single-file Water Transport Characteristics in Aquaporin-mimic Nanopores with O(100 nm) Length

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In this paper, we would like to present our researches that consist of two parts. First, we analyzed water permeation dynamics inside the super-long hour-glass water channel. For this research we designed a single file water channel model with 125, 150 and 175 Å in length. As the second research we have set a large scale water channel with three pore models as hour-glass, cylindrical and elliptical shapes with same length as 150 Å. For single file water channels we can observe: an interesting structure of water molecules around the narrowest section with varying the length, the formation of five discrete areas to density distribution along the length, incrementing of permeability and diffusivity by increasing the length, a good agreement between our permeability results and experiment results and the insignificant effect of changing the length on potential of mean force at center region. For large scale we found that water molecules leave the pore at the lowest average velocity through the elliptical pore, hour-glass and elliptical pores have the most water fluxes, cylindrical pore shows an anti-symmetric density distribution along the length and the most diffusivity and permeability happen via hour-glass and elliptical shaped pores. As our future plan we will analyze the slip length effect on fast water transport through single-file and large scale water channels. The previous investigations have shown this characteristic effects on fast water transport through artificial nanotubes. To this aim we intend to analyze that on super-long pores.

[1] G. Hummer, J.C. Rasaiah, J.P. Noworyta, Nature, 414, 188-190 (2001).
[2] S. Gravelle, L. Joly, F. Detcheverry, C. Ybert, C. Cottin-Bizonne, L. Bocquet, Proc. Natl. Acad. Sci. U. S. A., 110, 16367-16372 (2013).
[3] D. Tang, D. Kim, Appl. Therm. Eng., 72, 120-125 (2014).

VIP056
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Confined Impinging Nanofluids Slot Jets in Porous Media

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Heat transfer enhancement technology has the aim to develop more efficient systems as demanded in many applications in the fields of automotive, aerospace, electronic and process industry. A possible solution to obtain efficient cooling systems is represented by the use of confined impinging jets. Moreover, the introduction of nanoparticles in the working fluids can be considered in order to improve the thermal performances of the base fluids.

In this paper a numerical investigation on mixed convection in confined slot jets impinging on a purous media by considering pure water or Al_2O_3/water based nanofluids is described. A two-dimensional model is developed and different Peclet numbers and Rayleigh numbers were considered. The particle volume concentrations ranged from 0% to 4% and the particle diameter is equal to 30 nm. The target surface is heated by a constant temperature value, calculated according to the value of Rayleigh number. The distance of the target surface is five times greater than the slot jet width. A single-phase model approach has been adopted in order to describe the nanofluid behavior while the hypothesis of non-local thermal equilibrium is considered in order to simulate the behavior in the porous media which is featured by a porosity value of 0.87. The aim consists into study the thermal and fluid-dynamic behaviour of the system. Results show increasing values of the convective heat transfer coefficients for increasing values of Peclet number and particle concentration. This behaviour is more evident at low Peclet number values and Rayleigh number ones.

VIP059
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Displacement of Colloidal Dispersions in Porous Media: Experimental & Numerical Approaches
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The displacement of colloidal dispersions is of particular interest in many applications ranging from environmental issues to petroleum recovery. Natural porous media such as soils, aquifers or reservoirs contain colloidal particles of different nature (bacteria, viruses, clay, metal complexes …). Colloids can act as vehicles for micro organisms' transport in aquifers causing danger for human health. In petroleum recovery techniques, water containing colloids is sometimes injected and their release and adsorption may alter the petrophysical properties of reservoirs causing their damage. This talk focuses on the study of colloid transport in porous media under different hydrodynamic and physicochemical conditions (pH, salinity) using both experimental and numerical approaches. Typical laboratory experiments consist in the injection of a colloidal dispersion of a given concentration in a porous column. The analysis of the effluents after brine-flushing allows investigating the kinetics of release and adsorption of colloids inside the porous medium. In-situ investigations are performed either by post-mortem destructive methods or by using more sophisticated non-destructive methods. Moreover, a first approach to model these processes consists in solving the appropriate convection-dispersion-reaction equations involving macroscopic properties. Although this gives valuable qualitative insight on the displacement mechanisms, a more detailed study at the pore-scale is needed. Numerical approaches have been used at the pore-scale to study the displacement of colloidal particles. As a first approximation, the transport of the mass center of the particles has been considered. More complete numerical methods have allowed to study the transport of a colloidal particle taking into account pore-surface roughness, hydrodynamic forces and particle/pore physicochemical interactions (DLVO forces monitored through the change of the ionic strength of the suspending fluid). An overview of our experimental and numerical studies will be presented.

DSL360
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Identification of the Moisture Distribution in the Intensively Heated Porous Sand Mould
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The problem concerns the physical properties of the porous multi-component mould material to which the liquid metal is poured. In the mould quartz sand with bentonite binder the water is used to activate the physical mechanism of binding using bentonite. The technological water amount in so-called "green sand mould" does not exceed 4%. An important phenomenon accompanying the heating of this material by liquid metal (above 1000°C) is the production of water vapor and then its condensation in the so called "over-moisture zone" in the deeper layers of the mould relative to the metal contact surface.. This zone of moisture condensation is characterized by very low strength of mould sand and is the favorable factor to form the special casting defect (scab defect). In the over-moisture zone the local water content exceeds several times the value of initial technological moisture

content. Simultaneously the water evaporates increasingly when the temperature of mould is close to 100° C, the vapor is transported (presence of vapor pressure gradient), and further condenses in more and more distant (from casting) zones of the mould. This zone does getting more space and is moved into the mould to its external surface (contact with ambient).

The aim of the study is to determine the distribution of moisture in the intensively heated porous sand mould. In the past have been developed several measuring methods consisting in the water evaporation from a test sample (at given moment of time, the selected position coordinates of the sample), to determine an accumulated amount of water in the sample which is percentage of moisture content [1]. These methods provide a relatively good accuracy, but does not allow for the measurement of temporal continuity procedures during the dynamic process of moisture movement in the mould. The measurements performed by these methods allow the identification of points that allow the heated material moisture profile approximation for a given moment of time, but does not give the possibility of recording a dynamic movement of over-moisture zone. In some studies [2], in order to identify the distribution of moisture variation (as a function of distance and time coordinates) apply conductimetric method which uses the change of electrical conductivity of the sand mould with the change of its moisture. This method allows for the implementation of continuous measurements, but its disadvantage is the low accuracy, which allows the identification of the moisture only in the range from 2 to 10%. The study described in paper includes experiments of heating the green sand sample. Moisture distribution in the moisture transfer zone of the sample (temperature of the molding sand is approx. 100 ° C) was determined. In order to determine the moisture distribution an original method was used. This method allows interference in various layers of material of predetermined thickness, parallel to the surface of the mould of contact with a heat source. The classical measurement for determining moisture content of each layer was used. The moisture content of the test sample in over-moisture zone exceeds 10% (several times exceeds the initial moisture content).

[1] Dobosz S., Water in moulding sands and core moulding sands, Wyd. Naukowe AKAPIT, Kraków, 2006
[2] Szmigielski T., New version of a stand for testing resistivity of damp moulding sands, Archives of Foundry, Volume 6, № 22, 2006, pp 526–531

DSL208
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The Effect of Salt Solutions in the Capillarity Absorption Coefficient of Red Brick Samples

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Rising damp is one of construction's major problems associated with use of porous materials in this industry. This mechanism has a massive influence on the degradation of historical buildings since they were built in a time when construction technologies made no effort to prevent this kind of pathologies. The rising damp by itself can reduce the aesthetical value of the building and, when combined with the existence of soluble salts in the building and in the ground water can even lead to material decomposition and compromise the structural performance of the building. This happens due to the migration of the salt ions dissolved in water into the porous network of the building's walls where they remain and crystalize after water evaporates, dealing great pressures against the pore walls and eventually resulting in their fracture after many cycles of crystallization/dissolution.

The experimental work intended to study the effect of two different saturated solutions of sodium sulphate and potassium chloride in the capillary absorption curves obtained through the partial immersion of red brick samples. In the end of this paper there will be a macroscopic evaluation of the sample's crystallized top surface, obtained after a partial drying period. The results revealed significant differences in the capillary coefficients obtained when samples were tested with salt solutions.

DSL214
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Coupled Moisture and Temperature Caused Deformation of Innovative Plasters

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The problem of the reconstruction of the historical buildings surface layers is in material compatibility. To know some physical properties of materials is the basics for the appropriate choice of materials for reconstructions. The moisture and temperature induced deformations belong to these crucial physical properties.

The effect of temperature and moisture sorption on the elastic behavior of innovative plaster for renovation is investigated. From dilatation measurements (obtained at temperatures 20ºC and 60ºC) can be seen that material is deformed in the area of sorption moisture before reaching the state of intense capillary condensation and relative moisture elongation of material increases with moisture accrual. Thermodynamic analysis of the Clausius-Clapeyron relation provides the contributions of moisture and temperature caused expansion within coupled moisture and thermal deformation of plasters.

Special Session 8
FUNDAMENTALS TO APPLICATIONS IN 2D MATERIALS (SS8)

DSL243
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Morphological and Structural Characterization of Cu2ZnnS4 Thin Films Deposition by Ultrasonique Spray Pyrolysis

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Keywords: CZTS, spray technique, thin films, photoluminescence, Transmission, XRD, electrical conductivity.

The influence of substrate temperature on the properties of Cu2ZnSnS4 thin films elaborated by spray ultrasonic method has been investigated. Samples are deposited at various substrate temperature ranged from 280 to 360 °C about 45 min. the results of X-ray diffraction analyses indicated that Cu2ZnSnS4 films have nanocrystalline structure with (112) preferential orientation and reveals the formation of ZnSnO3 and Cu2ZnSnS4 phases. The crystalline size is varied from 20 to 45 nm with increasing substrate temperature. The optical films characterization was carried out by the measurement of UV-visible transmission. The optical gap was deduced from the absorption spectra. The photoluminescence spectrum measured at 77 K showed a broad emission around 1.27 eV. Electrical conductivity of the films is found to lie in the range 9 to 43 $(\Omega cm)^{-1}$.

DSL201
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Synthesis and Characterization of Hexamethyldisiloxane thin Films as Humidity Sensors

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Keywords: Hexamethyldisiloxane; Thin film; Humidity sensors; Electrical characterization.

This paper reports the study of electrical properties of plasma polymerization of hexamethyldisiloxane (pp-HMDSO) thin film based sensors. Thin water molecule sensitive layers were deposited from hexaméthyldisiloxane precursor on tow-interdigited electrode at low frequency power (19 KHz) plasma conditions. The sensor was calibrated in terms of impedance as a function of relative humidity, using a Frequency Response Analyzer. The electrical properties of the sensor are measured. The deposited film sensor exhibited a accepted sensitivity (impedance change from 106 to 104 Ω in the humidity range of 30–95% RH), fast response (8 and 34 s for adsorption and desorption between 35% RH and 95% RH, respectively) [1-2], and the current intensity increased from 10-10 to 10-6 A in the explored range of RH (25-95% RH). The change in the current of pp-HMDSO with respect to increasing and decreasing RH (hysteresis) of no more than 4% has been observed. Structural analysis of the sensitive layer was carried out by Fourier Transform Infrared spectroscopy (FTIR). The films showed good sensitivity to water molecule due to the presence of hydroxyl groups OH. These groupments provide the adsorption

sites for water and play an important role in the humidity sensor properties, make the elaborated layer a promising candidate for humidity sensors devellopement.

References:
[1] N. Guermat, A. Bellel, S. Sahli, Y. Segui, P. Raynaud, "Thin plasma-polymerized layers of hexamethyldisiloxane for humidity sensor development", Thin Solid Films, vol 517, pp. 4455–4460, 2009.
[2] N. Guermat, A. Bellel, S. Sahli, Y. Segui, P. Raynaud, "Plasma Polymerization of Hexamethyldisiloxane and Tetraethoxysilane Thin Films for Humidity Sensing Application", Defect and Diffusion Forum, Vol. 354, pp 41-47, 2014.

VIP014
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Strain-induced Defects at Epitaxial Graphene/Silicon Carbide Surface and Interface

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Graphene is a single atomic layer of graphite. It could be exfoliated from graphite, or grown by CVD/MBE methods on metal, semiconductor or insulating substrates. It could also be grown epitaxialy on the surface of a wide band gap semiconductor, silicon carbide (SiC), an especially suitable substrate for epitaxial graphene growth. Graphene has outstanding and very promising properties, with figures of merit scaling well above those of well-established semiconductors [1]. Defects, nano-cracks and nanostructures at graphene/SiC surfaces/interfaces are investigated using advanced experimental techniques such as Synchrotron Radiation-based Photoemission Spectroscopy - SR-PES, Low Energy Electron Microscopy - LEEM, μ-spot X-Ray Photoemission Spectroscopy - μ-spot XPS and Scanning Tunneling Microscopy/Spectroscopy - STM/STS. Strain and/or stress are the driving forces in SiC substrate surface/interface organization, leading to complex surface atomic structures and nano-objects. Depending on growth conditions, these factors result in defect formation including: i) atomic cracks developing on the SiC substrate, ii) nano-objects resulting from the growth of carbon-nanotubes (CNT) at graphene/SiC interface and iii) graphene ripples. As evidenced by STS and SR-PES, the CNTs at the graphene/SiC interface lead to electronic interface states (EIS) (in agreement with ab-initio FLAPW calculations) that could be detrimental to the transport properties. Interestingly, the graphene layer is found to go deep into the nano-cracks without any disruption or resulting EIS, in strong contrast to the CNTs. The different mechanisms at the origin of these features will be presented and discussed. The results directly impact the monitoring of graphene/SiC surface/interface properties.

[1] "Graphene: Fundamentals and Functionalities", W. Lu, P. Soukiassian, J. Boeckl, Guest Editors of MRS Bulletin 37 Special Issue, p.1119-1321 (2012); "Will Graphene be the Material of the 21th Century?", P. Soukiassian, MRS Bulletin 37, 1321 (2012).

VIP015
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Synthesis of Graphene on Silicon

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Graphene is currently one of the most promising nanomaterials, thanks to the extraordinary physical, electronic and mechanical properties of its pristine form. Nevertheless, the full understanding and control of its properties, and the unlocking of its large potential for micro– and nanodevices, have been hindered so far by the lack of a reliable method to obtain structured graphene in a controlled and reproducible fashion. This would be best achieved at the wafer- level. The only feasible wafer-level route to–date is based on the use of SiC wafers to obtain high-quality graphene from Si sublimation in the 1300-1600°C temperature range [1]. However, prohibitive costs associated to the use and processing of SiC wafers are a major limitation. Attempts to produce wafer-scale graphene through sublimation from the cheaper SiC epitaxial layers on Si wafers have been reported [2]. Invariably, the quality of such graphene has been significantly inferior to that obtained from SiC wafers. We have explored the use of epitaxial SiC on silicon as substrate for wafer–level graphene through the use of metal catalysts and direct decomposition. We report for the first time in literature the achievement of high–quality graphene around 1050°C with a controlled number of layers on epitaxial SiC on Si by adjusting the ratio of a Ni:Cu alloy catalyst film [3]. As the few–layers–graphene is obtained at the SiC/metal interface, the catalytic layer can be removed via wet etch, leaving behind the graphene on SiC ready to be used in a device with no need for manual transfer. This finding opens the first realistic avenue to a mass production of graphene devices and their integration with the mainstream electronic systems in CMOS technology.

[1] Walt A. de Heer, Claire Berger, Ming Ruan, Mike Sprinkle, Xuebin Li, Yike Hu, Baiqian Zhang, John Hankinson, and Edward Conrad, PNAS, 108 (2011) 16900.

[2] H. Fukidome, Y. Kawai, H. Handa, H. Hibino, H. Miyashita, M. Kotsugi, T. Ohkochi, M. Jung, T Seumitsu, T. Kinoshita, T. Otsuji, and M. Seumitsu, Proc. IEEE, 101 (2013) 1557.

[3] F. Iacopi, B.V. Cunning, and M. Ahmed, September 2013, patent pending.

VIP067
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Optoelectronics in Van Der Waals Heterostructures

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Building on the tremendous developments in graphene studies, van der Waals (vdW) heterostructures have been recently envisioned as defect-free stacks of different atomically-thin layered materials to combine their various physical properties [1]. This paradigm shift opens the path to the elaboration of original flexible and transparent electronics with superior performance. Among these 2d-materials, transition metal dichalcogenides (TMDs) have been successfully implemented as the semiconducting active layer in devices such as vertical transistors, photodetectors or light emitters [2]. In this talk I will discuss different schemes for photodetection that can simultaneously possess large active area, high efficiency, and fast response time. In particular I will focus on a vertical geometry where visible light is absorbed in WSe2 layers and photocreated charges are then collected through top and bottom graphene transparent electrodes. In this work we make use of time resolved photocurrent measurements and extract the timescales during which the photocarriers travel in the active region as function of its thickness and bias voltage [3]. We demonstrate high internal efficiencies coupled with short response times down to 6 ps. We describe the light-to-current conversion in terms of dissociation, drift and interlayer transfer of the photocarriers, in competition with recombination. The clear determination of the mechanisms and limitations

in such vertical geometry lays the groundwork for designing optimized future optoelectronic applications based on vdW heterostructures.

[1] A.K. Geim & I.V. Grigorieva, Nature 499, 419–25 (2013).
[2] L. Britnell et al., Science 340, 1311–4 (2013).
[3] M. Massicotte et al., submitted

VIP068
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On The Graphitization of Reducible and Irreducible Oxides and their Potential Applications
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The catalytic potential of metal catalysts, in particular transition metals, is well known. Indeed, they are frequently used in the synthesis of nanomaterials. For example graphene growth is usually fabricated over copper. However, despite the success of metal catalysts sometimes this can be a disadvantage. For example, when growing graphene over a metal, if it is to be used for device fabrication it needs to be transferred onto an insulator. This transfer process can be damaging. Thus, sometimes it is preferable to synthesize such materials directly over oxides. In this presentation a variety of synthesis approaches for 0D, 1D and 2D synthesis over oxides along with their characterization will be presented. Structures like graphitic shells (0D), carbon nanotubes/fibers (1D) and graphene (2D) are discussed using synthesis routes such as chemical vapor deposition (CVD) and carbothermal reduction. The potential for these materials to be used in applications for electronic, energy and bio-medical applications is also discussed.

VIP069
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2D Materials-Based Electronics: Where Do we Go from here?
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In this presentation, I will try to provide perspectives and challenges of 2D materials (2DMs) technology, which aims, in the best previsions, at becoming the benchmark technology for electronic applications [1]. In particular, I will first focus on digital applications, discussing the main figures of merit against technology requirements, showing the point of strength and of weakness, when exploiting 2DMs as channel material for next-generation devices. With respect to this, 2DMs heterostructures [2,3] will be also addressed, while proposing new device architectures. Radio frequency applications will be discussed [4,5], focusing on the performance expected in the

THz regime, and graphene transparent electrode as possible substitute for Indium Tin Oxide in organic solar cell will be investigated through numerical simulations.

[1] Gianluca Fiori, Francesco Bonaccorso, Giuseppe Iannaccone, Tomas Palacios, Daniel Neumaier, Alan Seabaugh, Sanjay K. Banerjee, Luigi Colombo,'Electronics based on two-dimensional materials' Nature Nanotechnology, Vol. 9, p. 768-779, 2014
[2] Fiori G, Betti A, Bruzzone S, Iannaccone G, 'Lateral Graphene-hBCN Heterostructures as a Platform for Fully Two-Dimensional Transistors' Acs Nano, Vol. 6, p. 2642-2648, 2012.
[3] G. Fiori,S. Bruzzone,G. Iannaccone, 'Very Large Current Modulation in Vertical Heterostructure Graphene/hBN Transistors' IEEE Transactions On Electron Devices, Vol. 60, p. 268-273, 2013
[4] Gianluca Fiori, Daniel Neumaier, Bart N. Szafranek, Giuseppe Iannaccone, 'Bilayer Graphene Transistors for Analog Electronics' IEEE Transactions On Electron Devices, Vol. 61, p. 729-733, 2014
[5] B.N. Szafranek, G. Fiori, D. Schall, D. Neumaier, H. Kurz, 'Current saturation and voltage gain in bilayer graphene field effect transistors' Nano Letters, Vol. 12, p. 1324-1328, 2012

VIP070
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Silicene and Germanene: Emerging Synthetic Two-Dimensional Electronic Materials

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Silicene and germanene are graphene's silicon and germanium synthetic analogues. In the last years, they have attracted considerable interest as novel Si and Ge 2D allotropes and emerging 2D electronic materials [1,2]. Since they do not exist in nature they are created artificially in situ in ultra-high vacuum on metal substrates. The recent fabrication of the first silicene FETs operating at room temperature demonstrates their potential for ultimate scaling of nanoelectronic devices [3].

In this talk, I will present the archetype 3x3 silicene phase formed on a silver (111) substrate [4], its sister phases and next the growth of multilayer silicene, which hosts Dirac fermions and which is stable in ambient air, protected by an ultra-thin native oxide [5]. The recent synthesis of germanene will be also discussed [6]. Finally, the applications envisaged with these novel 2D materials will be addressed.

[1] G. Le Lay, Nature Nanotechnology, published online Feb. 2, 2015.
[2] A. Dimoulas, Microelectronic Engineering, 131, 68 (2015).
[3] Li Tao et al., Nature Nanotechnolgy, published online Feb. 2, 2015.
[4] P. Vogt et al., Phys. Rev. Lett., 108, 155501 (2012).
[5] P. De Padova et al., 2D Mater., 1, 021003 (2014).
[6] M.E. Dávila et al., New J. Phys., 16, 095002 (2014).

VIP071
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Graphene Coatings for Alkali Resistance

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Atomic physics based devices are being developed that take advantage of the simple electronic structure of chemically active alkali-metal and alkali-earth elements. Due to the chemical activity of alkali atoms and often intense radiation, severe damage to optical elements in these systems occurs. This damage shortens the service life of alkali-based atomic physics devices. In order to prolong the lifespan of these systems, a need for alkali resistant optical coatings has arisen. Graphene holds promise for use as such a protective coating [1]. Graphene was produced by thermal decomposition of single-crystal SiC in ultrahigh vacuum [2-3]. These graphene films were exposed to Rb and Cs at 270 Psi at 250°C. Spectrophotometry, Raman spectroscopy, and X-ray photoelectron spectroscopy were performed before and after exposure to alkali metal vapors in order to assess how the graphene layers affected the damage caused by the alkali vapors. Raman G/D ratios were investigated to show the amount of damage, and high resolution C 1s spectra determined the chemical shifts in carbon on the surface. These chemical shifts indicated the relative amounts of defect sites within the graphene. Both the theoretical and experimental results of graphene are encouraging for its use as a protective optical coating in atomic alkali-based system [1]. Results will be discussed.

[1] Nanoscale, 4 (2012) 1749.
[2] J. Phys. Chem., C 116 (2012) 15342.
[3] J. Phys. D: Appl. Phys. 43 (2010) 374004.

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Interfacial Interactions of Liquid Metals Functionalized by Self-Assembled Monolayers in Microfluidic Devices

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Gallium liquid metal alloys (GaLMA) are one of the key components of emerging technologies in reconfigurable, flexible, and printable electronics. Surface properties of GaLMA play important roles in its application in reconfigurable devices, such as tunable radio frequency antennas and electronic switches. Reversible flow of GaLMA in microchannels of these types of devices is hindered by the presence of an oxide skin that forms spontaneously in ambient environment. The oxide film sticks to most surfaces leaving unwanted residues behind that can cause undesired electronic properties. This work demonstrates an effective method in the surface modification of GaLMA that enables its reversible flow in microfluidic systems. The GaLMA surface is functionalized by self-assembled monolayers (decylphosphonic acid) in-situ which allows the liquid metal to move in the microchannels as a plug. X-ray photoelectron spectroscopy, vibrational spectroscopy, and contact angle measurements of the functionalized GaLMA surface indicate strong bonding between the phosphonic acid linker and the surface oxide of GaLMA. The 'plug-like' behavior of the liquid metal is explained by the presence of a slip-layer created by the ethanolic solution at the interface of GaLMA and microchannel walls.

VIP013
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Covetics – A New Class of Materials Containing High Carbon Concentration

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Covetics is a hybrid that fuses nanocarbons with metal forming bonds that are stronger than graphene's sp^2 bonds. To create these new materials, J. Shugart, co-inventor and CEO of a company called Third Millennium Materials established in Dayton developed a new method of carbon catalyzation which uses molten metal and metal alloys as an ionizing medium. Covetics were found to respond to physical and mechanical loadings in a superior way than polymers or metals. They show improvement in thermal and electrical conductivity and yield strength, and resist corrosion and oxidation.
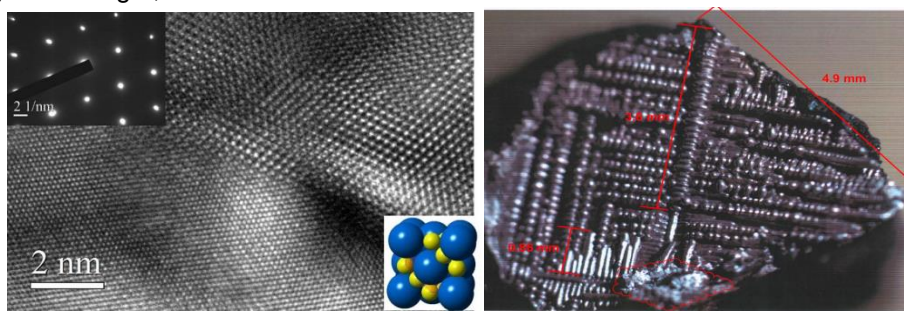
HRTEM and SEM images of covetics

Presentation has an informative character with intent to review briefly fundamental properties of covetics, to discuss atomistic scale bonding and structure of covetics based on the experimental characterization techniques (XRD, XPS, Raman and EELS), and to present the latest results of electrical and thermal measurements (ampacity) with plausible explanation of their unusual behavior.

Special Session 9
NANO/BIO MATERIALS SYNTHESIS, CHARACTERIZATION, MODELING AND APPLICATIONS (SS9)

DSL223
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The Effect of Treatment on Properties Thermomechanical Behavior of Poly (Vinylidene Fluoride) (Pvdf)

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The thin film of semi-crystalline poly (vinylidene fluorur) (PVDF) are subjected to tensile tests in plane strain in the temperature range (56 ° C to 115 ° C) and at different speeds by using the tensile test at videometric control (traction video) that is capable of giving the true stress and true strain.

The characterization of the various phases was made by the determination of the rate of crystallinity by using the techniques of DSC and x-rays.

Molecular mobility the material was observed by mechanical spectrometry while being focused on the study of the vitreous transition and structural relaxation.

The peak of relaxation β, associated to the low vitreous transition in the amorphous phase, shifts towards the high temperatures for stretched films, but annealing does not affect the position of this peak. This shows that the stretching plays a significant role in the phase transition. The intensity of this peak increases with these two treatments, this is due to the fusion of the small crystals in the amorphous phase. However the peak of relaxation β, associated to the molecular movements in the crystalline phase, moves towards the high temperatures because the rate of crystallinity of stretched and annealed films increases.

The relaxation β', associated to the high vitreous transition, increases with the increase of the temperature of annealing which means the increase of the interface which depends on the surface of the crystalline phase.

Key words: PVDF, tensile tests, relaxation.

DSL256
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Elaboration by Ground-Frost of Materials Photoniques Doped in Alkaline and Alcalino-Earthy

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Our diverse experimental tries(essays) allowed us to finalize(to work out) an optimal protocol for the obtaining of a material crystal clear and pure photonique by ground-frost. This synthetic plan was thought according to the sought(studied) physical properties and which were never approached. As precursors we used alcoxydes of silicon If (GOLD4) ;the acetic acide CH_3COOH being a chélatant and as solvent we used the ethylic alcohol C_2H_5OH and the water H_2O in well defined proportions. These frosts (gels) were doped by cations of alkaline metals (Na)

and alcalino-earthy (Ba and Sr) taken separatety and simultaneously.after ripening ;the analysis of the frosts (gels) obtained by diffraction in the X-rays (fig.1) shows a characteristic amorphous (apathetic) character which is translated by the appearance of domes of diffraction reflection of an atomic disorder . A thermal analysis and a spectrometry IR are envisaged .afin to observe the endothermic peaks of from solvents and from chélatant end to see the various bands (strips) of absorption of the present molecules in the frost (gel).

DSL266
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Clay Surface Modification by Vinyltrimethoxysilane (VTMS) Compound and Application in Synthesis of Polyurethane/clay Nanocomposites

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In this research Clay/ Polyurethane Nanocomposite was synthesized.The main problem for creation of this type of nanocomposites is the agglomeration of clay in Polymer Matrix which is related to the hydrophilic nature of clay which also causes stress concentration and reduction of mechanical properties in Clay/polyurethane nanocomposites. Then the Surface modification of clay minerals which is the purpose of this research therefore the silanization reaction was used. Vinyltrimethoxysilane (VTMS) was used as a coupling agent for surface modification of clay[1].to prepare the samples, determined amount of modified and unmodified clay, prepared polyol , isocyanide(HDI) were stirred, sonicated and vacuumed then were poured in silicon mold to cure the samples. Furthermore, The Analysis including FT-IR, XRD, SEM, and TEM shows that using this compound as a modifier can increase interlayer space of clay structure and lead to well dispersion of nanoclay in polymer matrix. The result of Mechanical analysis data of polyurethane/Clay nanocomposites shows that, adding a small amount of modified clay in polyurethane matrix leads to improvement of mechanical properties,sach as increase of module and tensile strength.

Keywords: Nanocomposite, Clay, Polyurethane, Surface modification, Silane

[1] H. Zhou, Y. Su, X. Chen, S. Yi, Y. Wan, Separation and purification technology, 75, 286, (2010)

DSL284
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Crystal Growth of Metal Oxide by Reaction of Metal Chloride with Surface of Cellulose

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We present a new approach of the preparation of the metal oxide from biotemplate in which the non-solubilized cellulose is treated in anhydrous condition with solution of metal chloride. Therefore, the formation of the metal oxide is the results of the reactivity of the cellulose acting as both an oxygen-donor and a template; several examples will be given like TiO_2, Nb_2O_5 or WO_3. Beside its originality this mineralization process of cellulose gives the access to original nano-sized morphology, in the absence of any structure directing agent (see pictures). The main issue related to this process and the morphology of the nanostructures, is the questions on the diffusion of the reagent through the cellulose fiber and the growing of the metal oxide crystals at the Solid (cellulose)/Liquid(metal chloride in solvent) interface. Following our proposition, discussion and suggestions will be welcome.

[1] G. R. Nair, S. K. Samdarshi,and B. Boury European Journal of Inorganic Chemistry 5303–5310 (2013)
[2] B. Boury and S. Plumejeau Green Chem., 17, 72-88 (2015)

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Asymmetrical self-Diffusion with Orientation-Dependence of Molecules on Finite Timescale
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Using molecular dynamics simulations, we show that self-diffusion of a nanoscale particle (molecule) with asymmetric structure critically depends on the orientation in a finite time of picoseconds to nanoseconds. In a timescale of 100 ps, there are about 10% more possibilities for the particle moving along the initial orientation than moving opposite to the orientation; and the diffusion distances of the particle reach about 1 nm. We find that the key to this observation is the orientation-dependence of the damping force to the moving of the nanoscale particle and a finite time is required to regulate the particle orientation. Our finding provides significant insights into the fundamental understanding of biological processes in relation to the diffusion of biomolecules in living cells and of nanoparticles in various nano-systems, which usually happen in a finite time.

[1] N. Sheng, Y. S. Tu, P. Guo, R. Z. Wan, and H. P. Fang, Sci. China Phys. Mech., 56, 1047 (2013).

VIP062
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Formation of Bio-Compatible Titanium Di-Oxide Layer Onto 316L Stainless Steel Substrate
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Present study focuses on improving biocompatibility of biomedical 316L stainless steel at low processing temperature while preserving its high mechanical performance. In that respect, sequential application of cold dynamic gas spraying and micro arc oxidation processes on 316L substrate generated biocompatible compounds containing titanium oxide layer and titanium inner layer beneath it. Titanium coating was produced by cold spraying method because of its low processing temperature and dense microstructure. Micro arc oxidation was employed in an electrolyte containing calcium and phosphorous species in order to incorporate biocompatible compounds into the oxide coating while titanium surface was oxidized. Microstructural investigations, X-Ray diffraction analysis, hardness measurements, wear and in vitro bioactivity test were utilized for the characterization of the coating.

VIP073
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Complex Metallic Alloys as Novel Reinforcing Agents in Biocompatible Polymer Matrix Nanocomposites

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Complex metallic alloys (CMAs), are new class of intermetallic compounds with complex crystal structure and giant unit cells as well as large lattice parameter. These materials have good potential for using either in single or polycrystalline bulk form, as coatings on various substrates, or as dispersion of particles in a metallic or polymeric matrix for different possible technical applications. Recently we succeed to prepare single phase CMAs such as $Al_{12}Mg_{17}$ compound by homogenizing annealing heat treatment [1].

Polymer/CMA nanocomposites can be applied for structural and biomedical demands. Polyetheretherketone (PEEK) is a semi-crystalline biocompatible thermoplastic polymer with excellent physical and mechanical properties such as high strength, modulus toughness and wear resistivity. Due to its unique characteristic, PEEK is of central interest in industrial and biological applications. In our previous study [2], effect of Al_3Mg_2 CMA nanoparticles addition on the microstructure of PEEK nanocomposite samples prepared by mechanical milling and hot pressing was presented. Considerable strengthening can be achieved by adding CMA particles to PEEK matrix through uniform distribution of nanoparticles. Novel polymer matrix nanocomposites reinforced with complex metallic alloys (CMAs) are discussed in this research.

[1] A. Zolriasatein and A. Shokuhfar, J. Mater. Design, 75, 17 (2015).
[2] A. Zolriasatein, A. Shokuhfar and M. Alzamani, J. PROC.NAP., 1, 03CNN20 (2012).

DSL200
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Measurement of Mass Diffusivity of an Aqueous Laponite Suspension Using Laser Interferometry

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Mass diffusion of a solute in a solvent is realized in many applications. Refractive index techniques for determination of mass diffusion coefficient of a solute in a binary system have many advantages as discussed in the literature [1, 2]. The extraction of transport properties of colloidal suspensions from optical images has not received sufficient attention. The issue becomes important when refractive index is a strong function of solutal concentration and thermal diffusivity is small.

Mass diffusivity of an aqueous suspension of disk shaped nanoparticle of Laponite JS in tetra-sodium pyrophosphate solution at different concentrations and temperatures is studied using laser interferometry. Laponite JS makes a transparent colloidal suspension (sol forming grade) when dispersed in deionized water maintained at pH 10. It is a colloidal synthetic layered silicate composed of platelets having an oblate shaped particle of diameter 25 nm and a thickness of 1 nm. During an experiment, a layer of suspension is placed in a temperature-controlled cavity with tetra-sodium pyrophosphate solution above. The interference pattern formed due to the diffusion of solute into solventr above leads to the formation of time-dependent fringe patterns. Fringes are analyzed to determine the mass diffusivity of the solute in the solvent. A similar study of thermal diffusivity was reported by the authors earlier [3].

From the results obtained, a substantial enhancement of mass diffusivity is seen for a small increase in the amount of Laponite in water at a given temperature. The joint dependence of mass diffusivity on concentration and temperature is more complicated. Surprisingly, at specific concentrations, the mass diffusion coefficient is observed to decrease with increase in temperature. Independently, the measurement approach described above should be a useful tool for studying transport phenomena in the colloidal suspensions, including the biological solutions.

[1] E. Kaunisto, M. Marucci and A. Axelsson, AIChE Journal, 57(10), 2610 (2011).
[2] A. Koniger, B. Meiery and W. Kohler, Philosophical Magazine, 89(10), 907 (2009).
[3] S.S. Bhandari, K. Muralidhar and Y.M. Joshi, Ind. Eng. Chem. Res., 52, 15114 (2013).

DSL324
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Recycling of Policarbonate Waste from Automotive Industry by Blending it with ABS to Compose ABS/PC Alloys

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This study proposes the production and characterization of blends of ABS/PC through reuse of discarded PC in the automotive panel production process [1]. The developed alloy ratios are (ABS/PC) 30/70, 50/50 and 70/30, in addition to the neat materials. The chemical composition of the neat ABS used in the alloy is 50-70 wt% acrilonitrile, 10-30 wt% SAN, 10-30 wt% ABS e <0,2 wt% styrene, according to the Safety Data Sheet provided by the manufacturer. The blends were processed in a twin screw extruder under controled heating temperature. One of the uses of the polycarbonate in the automotive industry regards the foils applied to the panel. These foils added up with other plastic parts made of several resins, e.g. ABS, ABS/PC, PP, PMMA compose the vehicle cockpit. The foil manufacturing starts with the acquisition of the cast polycarbonate film and is followed by the graphical part applied by printing process, which is conceptually defined as the superficial deposit of ink layers, and concluded with the cut of parts and disposal of wastes. All along this process, the material does not go through any situation that might reduce or change the integrity of the chemical and physical properties of the PC raw material. The printed parts use about 70% of the film area and the remaining 30% is disposed as plastic flaps together with defective parts coming from the same manufaturing process. Regarding the recycling process, the

material is handled in a clean room which eliminates the need of washing or any other cleaning process to adjust the material to be reused. A chemical process to remove the ink from the PC is not recomended not only for the high cost but also for the generation of harmful waste to the environment. Thus, the material must move forward to another process cycle with no intervention. In this case, the recycling is made by mechanical crushing of the film waste that will subsequently be reused in the extrusion molding process (pelletizing) together with the neat ABS composing the ABS/PC alloy. This alloy presents two important properties for automotive applications: improved melting flowability considering the neat PC as reference and increase in the notched impact strength due to mixing with ABS. This latter property is closely linked to the ABS morphology and related to the dispersion of rubber in the SAN matrix of the resin. Studies related to recycling and recovering of WEEE (Waste Electrical and Electronic Equipment) [2,3] show that there is a limit in the polymer reuse after processing. Both ABS and ABS/PC recicled through this kind of process become a percentage in the new resin mixture composition being used as a ratio of the neat material or need to be compatibilized with a SAN-g-amine to reach better rubber dispersion.

In case of ABS/PC made with foil recycled polycarbonate, the effects of inorganic material (ink) deposited on the surface are measured by using different mechanical characterization techniques (Stress Strenght, Flexural, Toughness and Notched Izod Impact Strength), thermal tests (TGA, HDT, Vicat) and rheological tests (Melt Index Flow, Dynamic Mechanical Analysis) to analyse the compatibility and the physical properties of the alloy, in addition to the use of Scanning Electron Microscopy to observe the material morphology.

[1] A.A. Zorpas, V.J. Inglezakis, J. Tech.Soc., 34, 55 (2012).
[2] R. Scaffaro, L. Botta, G. Di Benedetto, J. Eur.Polym., 48, 637 (2012).
[3] R. Balart, J. López, D. García, M.D. Salvador, J. Eur.Polym., 41, 2150 (2005).

DSL326
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Rotational and Translational Diffusion of Admixture Molecules in Liquid Crystals Determined by EPR Spectroscopy

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Rotational and translational diffusion of the series of stable nitroxide radicals in nematic and smectic mesophases was investigated by means of EPR spectroscopy. Characteristics of rotational mobility of the radicals were estimated by numerical simulation of the shape of their EPR spectra. It was found that mechanism of rotation of the probes in liquid crystals is essentially differs from rotation in unstructured matrixes and can not be described as Brownian diffusion. Radicals with sufficiently nonaxial inertia properties rotate fast around one axis and vibrate around perpendicular ones. Also it was shown that chemically identical admixture molecules in liquid crystal matrices can have different rotational properties. Rotation diffusion coefficients for such particles can differ by an order of magnitude. This fact indicates various localization of admixture molecules in liquid crystalline media. Coefficients of translational diffusion of the radicals were found by analysis of concentration broadening of EPR spectra reflecting their spin exchange interactions. The results are compared with the data obtained by other methods.

DSL354
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Separation of Sulphuric Acid from an Acid Suspension of Cellulose Nanocrystals by Manual Shaking

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In this work, a separation method of sulphuric acid from a suspension of cellulose nanocrystal by manual shaking is described. Cellulose nanocrystals are prepared from acid hydrolysis of cotton using 64 wt% sulphuric acid at ca. 45°C for 45 minutes. After the hydrolysis was complete, water was added to dilute the mixture to a resulting concentration of 30 wt% of the acid. This mixture was shaken rigorously in a closed container and after 48 hours, separation occurs such that the cellulose nanocrystals, which had higher density than the 30 wt% sulphuric acid, float with the bubbles introduced by the shaking. As a result of the floating of the cellulose nanocrystals, clear acid solution can be collected at the bottom of the container. The phenomenon of floating cellulose nanocrystals is discussed, and a phenomenological model for the process is suggested based on the results of this work. This shaking-floating process is repeatable for several cycles after the acid was removed from the bottom and more water was added. Using this simple process, the total acid recovery of > 90% has been achieved, and the concentration of all the acid recovered combined was 17.5 wt%.

DSL355
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Syntheses and Characterization of Potential Drug Carrier Nanocomposites

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The core-shell nanoparticles (CSNPs) [1] are widely used for therapy and diagnosis to deliver a drug in the right place at the right time in the adequate concentration [1]. The main biological requirements for the synthesis of CSNPs: utilization of biodegradable and biocompatible materials without immunogenic and thrombogenic features. The suitable CSNPs have a diameter below 100 nm and are stable in blood during prolonged circulation time. Many potential therapeutic agent using in biological systems are limited namely they can't get through the BBB, this owing to their properties, for examples size, liophilicity, charge, etc. This barrier could be eliminated by chemical modifications, interactions with other molecules or application of composites. Novel, carrier-systems in nanoscale may promote the drug delivery into the brain which give possibility to treat the neurological disorders [2]. For this purpose we have synthetized one-layered core-shell nanocomposite for delivery of different drug molecules like kynurenic acid, dopamine and ketoprofen. The size and the structure of the prepared nanocomposites have been investigated by dynamic light scattering (DLS), CD spectroscopy, high resolution transmission electron microscopy (HRTEM) and small angle X-ray scattering (SAXS) techniques. In order to study the interaction between the chemical components of nanocomposites (e.g. proteins, polymers, polysaccharides, drug molecules) two-dimensional sensor techniques like surface plasmon resonance (SPR) and reflectometry interference spectroscopy (RIfS) have been used. Because the SPR measurements were carried out at different temperatures (from 10°C to 40°C) we provided important information about the thermodynamic state functions of

the interactions besides the quantitative binding data [3]. The release of the drug molecules were controlled by desorption measurements. In vitro BBB model was used to study the drug penetration through the blood-brain barrier by CSNPs. Based on the results of in vitro and in vivo experiments this nanocarrier system may the future of brain drug development.

[1] N. Varga, M. Benkő, D. Sebők, I. Dékány, Colloids and Surfaces B: Biointerfaces, 123, 616 (2014).
[2] R. Alyautdin, I. Khalin, M.I. Nafeeza, M.H. Haron, D. Kuznetsov, International Journal of Nanomedicine, 9,795 (2014).
[3] E. Csapó, Z. Majláth, Á. Juhász, B. Roósz, A. Hetényi, J. Tajti, G.K. Tóth, L. Vécsei, I. Dékány, Colloids and Surfaces B: Biointerfaces, 123, 924 (2014).

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Structural and Transport Properties of Rare Earth Oxide-Cu-Ni-Ag Systems

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Transport and mechanical properties of copper based alloys can be improved by using rare earth oxides in their composition, so these cermets have potential technological application from cutting tools up to fuel cell devices [1]. Besides the mechanical resistance and hardness improvement, such oxides also minimize high radio-frequency fields, and thus current density increases [2]. In this work lanthanum and cerium oxide were used in Cu-Ni-Ag alloy as metallic matrix [3,4], so that four different compositions were obtained by powder metallurgy. After mixing in reactive milling and casting under cold pressing at 40kgf/cm2, the samples were sintered in vacuum during 7 hours at 700°C. Samples were characterized by Optical Microscopy (OM), Scanning Electron Microscopy (SEM), X-Ray Diffraction (XRD), Rietveld-Le Bail Refinement (RR), Vickers Hardness Test (VHT) and Four Point Resistivity Measurements (FPRM) by using a milliohm-meter. OM and SEM have shown high homogeneity of the ceramic particles, and the micrographies also indicate that the sintering process was efficient. XRD and RR results showed the complete solubilization of nickel into the copper matrix, but with some clusters. Rwp and Goodness of fitness parameters achieved in RR were 3.75 and 0.94, respectively. It was also observed the presence of silver precipitates, and it is according to the observed microstructures presented in the micrographies. In addition, according to the XRD and RR results, diffusion phenomena between ceramic and metallic matrix was evidenced by the presence of Ni-Ce intermetallic compound. VH measurements were carried out on the different phases and all the results are in agreement with the theoretical values. In the metallic matrix the higher value for VH was obtained for the nickel clusters. FPRM results indicate that the increasing in silver content slightly contributes negatively to the conductivity.

References
[1] Hong, Hyun Seon; Chae, Ui-Seok; Choo, Soo-Tae; Hendriks, Kyung Sub; Maria, Mark Gerard. Microstructure and electrical conductivity of Ni/YSZ and NiO/YSZ composites for high-temperature electrolysis prepared by mechanical alloying. Journal of Power Sources, 2005, vol 149, p 84-89;
[2] Monteiro, Waldemar; Carrió, Juan Alfredo. Comportamento Elétrico E Mecânico De Ligas Metálicas Ternárias À Base De Cobre, Níquel Obtidas Por Metalurgia Do Pó. Universidade Presbiteriana Mackenzie, São Paulo, 2010;
[3] Monteiro, W. A., A. K. Okazaki, C. R. Da Silveira, J. A. G. Carrió, M. A. Carvalhal, And M. V. S. Surmani Martins. Sintering Of Ternary Copper Alloys (Powder Metalurgy)-Electrical And Mechanical Properties Effects. Intech Open Access Publisher, 2013;

[4] Okazaki, Anderson Kenji; Surmani Martins, Marcos Vinícius; Carvalhal, Marcelo De Almeida; Monteiro, Waldemar Alfredo; Carrió, Juan Alfredo Guevara. "Mechanical And Structural Characterization Of Cu-Ni-Ag/Y2o3 Composites Obtained By Powder Metallurgy." In Materials Science Forum, Vol. 727, Pp. 314-319. 2012.