

18<sup>th</sup> INTERNATIONAL MULTIDISCIPLINARY  
SCIENTIFIC GEOCONFERENCE  
SGEM 2018

CONFERENCE PROCEEDINGS  
VOLUME 18

Nano, Bio, Green and Space -  
Technologies for a Sustainable Future

Issue: 6.1



MICRO AND NANO TECHNOLOGIES  
SPACE TECHNOLOGIES AND PLANETARY SCIENCE

**18<sup>th</sup> INTERNATIONAL MULTIDISCIPLINARY  
SCIENTIFIC GEOCONFERENCE  
S G E M 2 0 1 8**

**CONFERENCE PROCEEDINGS  
VOLUME 18**



**NANO, BIO AND GREEN – TECHNOLOGIES  
FOR A SUSTAINABLE FUTURE  
ISSUE 6.1**

-----  
**MICRO AND NANO TECHNOLOGIES,  
SPACE TECHNOLOGIES AND PLANETARY SCIENCE**  
-----

**2 July - 8 July, 2018  
Albena, Bulgaria**

---

## DISCLAIMER

This book contains abstracts and complete papers approved by the Conference Review Committee. Authors are responsible for the content and accuracy.

Opinions expressed may not necessarily reflect the position of the International Scientific Council of SGEM.

Information in the SGEM 2018 Conference Proceedings is subject to change without notice. No part of this book may be reproduced or transmitted in any form or by any means, electronic or mechanical, for any purpose, without the express written permission of the International Scientific Council of SGEM.

Copyright © SGEM2018

All Rights Reserved by the International Multidisciplinary Scientific GeoConferences SGEM  
Published by STEF92 Technology Ltd., 51 "Alexander Malinov" Blvd., 1712 Sofia, Bulgaria  
Total print: 5000

ISBN 978-619-7408-50-8

ISSN 1314-2704

DOI: 10.5593/sgem2018/6.1

INTERNATIONAL MULTIDISCIPLINARY SCIENTIFIC GEOCONFERENCE SGEM  
Secretariat Bureau

E-mail: [sgem@sgem.org](mailto:sgem@sgem.org) | URL: [www.sgem.org](http://www.sgem.org)

## ORGANIZERS AND SCIENTIFIC PARTNERS

- THE CZECH ACADEMY OF SCIENCES
- LATVIAN ACADEMY OF SCIENCES
- POLISH ACADEMY OF SCIENCES
- RUSSIAN ACADEMY OF SCIENCES
- SERBIAN ACADEMY OF SCIENCES AND ARTS
- SLOVAK ACADEMY OF SCIENCES
- NATIONAL ACADEMY OF SCIENCES OF UKRAINE
- INSTITUTE OF WATER PROBLEM AND HYDROPOWER OF NAS KR
- NATIONAL ACADEMY OF SCIENCES OF ARMENIA
- SCIENCE COUNCIL OF JAPAN
- EUROPEAN ACADEMY OF SCIENCES, ARTS AND LETTERS
- ACADEMY OF SCIENCES OF MOLDOVA
- MONTENEGRIN ACADEMY OF SCIENCES AND ARTS
- CROATIAN ACADEMY OF SCIENCES AND ARTS, CROATIA
- GEORGIAN NATIONAL ACADEMY OF SCIENCES
- ACADEMY OF FINE ARTS AND DESIGN IN BRATISLAVA
- TURKISH ACADEMY OF SCIENCES
- NIZHNY NOVGOROD STATE UNIVERSITY OF ARCHITECTURE AND CIVIL ENGINEERING, RUSSIAN FEDERATION
- BULGARIAN ACADEMY OF SCIENCES
- BULGARIAN INDUSTRIAL ASSOCIATION
- BULGARIAN MINISTRY OF ENVIRONMENT AND WATER

## INTERNATIONAL SCIENTIFIC COMMITTEE

### Nano, Bio, Green and Space - Technologies for a Sustainable Future

- PROF. STEFAN DIMOV, UK
- PROF. MARIAPIA VIOLA MAGNI, ITALY
- PROF. STEFFEN LEHMANN, AUSTRALIA
- PROF. RAJAT GUPTA, UK
- PROF. DI MAAS PETER DROEGE, LICHTENSTEIN
- PROF. NIKOLOZ CHIKHRADZE, GEORGIA
- PROF. JAN KAZMIERCZAK, POLAND

- PROF. VADIM ZHMUD, RUSSIA
- DR. FRANCIS BALESTRA, FRANCE
- DR. ANDROULA NASSIOPOULOU, GREECE
- ASSOC. PROF. KRYSZYNA JANUSZKIEWICZ, POLAND
- DR. EMILIO MIGUEL MITRE, SPAIN
- PHD. SINISA SRECEC, CROATIA

---

**CONFERENCE PROCEEDINGS CONTENTS**


---

**MICRO AND NANO TECHNOLOGIES**


---

- 1. A COMPUTATIONAL METHOD FOR THE PREDICTION OF CORROSION RESISTANCE OF SOME IRON POWDER METALLURGY MATERIALS,** Mihaela Marin, Florin Bogdan Marin, Dunarea de Jos University of Galati, Romania ...3
- 2. A FEW ASPECTS CONCERNING THE INFLUENCE OF THE ELECTRODES ON THE SF<sub>6</sub> INSULATION DIELECTRIC BEHAVIOR,** Adrian Paun, Flaviu Mihai Frigura-Iliasa, Mihaela Frigura-Iliasa, Petru Andea, Doru Vatau, Politehnica University Timisoara, Romania.....9
- 3. ALTERNATIVE NON-DEMOUNTABLE ASSEMBLY TECHNOLOGIES FOR ALUMINUM ALLOYS,** Dimitrescu A, Babis C, Alecusan AM, Chivu O, Ungureanu L, University Politehnica of Bucharest, Romania .....17
- 4. AN ORIGINAL CAD BASED DESIGN FOR A DOMESTIC LOW VOLTAGE SURGE ARRESTER MODULE,** Emil Lazarescu, Mihaela Frigura-Iliasa, Lia Dolga, Hannelore Filipescu, Madlena Nen, Politehnica University of Timisoara, Romania .....25
- 5. ANALYSIS OF WEARABLE INTELLIGENT DEVICES FOR INCREASED SAFETY IN HAZARDOUS ENVIRONMENTS,** Dr. Eng. Suciuc, G., Pasat, A., Nadrag, C., Balanescu, M., BEIA Consult International, Romania .....31
- 6. ANTI-CORROSION PROPERTIES OF NANOCOMPOSITE COATINGS IN AMINE ENVIRONMENTS,** Prof. DrSc Kanat Mukashev, PhD-student Rustem Atchibayev, Prof. Abyl Muradov, Dr Ainur Kyzzyrova, Dr Zhasulan Aitbayev, Al-Farabi Kazakh National University, Kazakhstan.....39
- 7. ANTIBACTERIAL POLYMERIC NANOCOMPOSITES BASED ON PVC AND FUNCTIONALIZED TiO<sub>2</sub> NANOPARTICLES WITH APPLICATION IN THE MEDICAL AND FOOD INDUSTRIES,** GEORGESCU MIHAI, ALEXANDRESCU LAURENTIA, SONMEZ MARIA, NITUICA MIHAELA, FICAI ANTON, INCDTP-Div. Leather and Footwear Research Institute ICPI, Romania.....47
- 8. APPLICATION OF AN ARTIFICIAL NEURAL NETWORK FOR PREDICTION OF THE WEAR RESISTANCE OF SINTERED IRON ALLOYS,** Florin Bogdan Marin, Mihaela Marin, Dunarea de Jos University of Galati, Romania.....55
- 9. APPLICATION OF PALLADIUM-CONTAINING POLYSTYRENE-BASED MAGNETICALLY SEPARABLE CATALYSTS IN FINE ORGANIC SYNTHESIS,** Prof. Esther Sulman, Dr. Oleg Manaenkov, Mrs. Nadezhda Nemygina, Dr. Linda Nikoshvili, Prof. Lioubov Kiwi-Minsker, Tver Technical University, Russia .....61

48. **OBTAINING COMPOSITE MATERIALS OF THE POLYMER-ALUMINUM TYPE BY GLUING USING BICOMPONENT ADHESIVES**, Dr. Dimitrescu A, Dr. Babis C, Alecusan AM, Dr. Chivu O, Dr. Ungureanu L, University Politehnica of Bucharest, Romania .....355
49. **ON DEFORMATION BEHAVIOUR AND MICROSTRUCTURAL CHANGE OF Cu-9.51Al-3.81Ni ALLOY**, Gheorghe Gurau, Carmela Gurau, Dunarea de Jos University of Galati, Romania.....363
50. **OPERATING CHARACTERISTICS OF CONCRETE MODIFIED BY HIGH-DISPERSED SAPONITE-CONTAINING MATERIAL**, Marina Morozova, Associate Professor Maria Frolova, Professor Valeriy Lesovik, Professor Arkady Ayzenshtadt, Northern Arctic Federal University, Russia .....371
51. **OPTIMIZATION OF SOLUBILITY OF AMIODARONE HYDROCHLORIDE THROUGH COMPLEXATION WITH HYDROXYPROPYL- $\beta$ -CYCLODEXTRIN**, Andreea Creteanu, Alina Stefanache, Gladiola Tantar, Madalina Vieriu, Lacramioara Ochiuz, Gr. T. Popa University of Medicine and Pharmacy, Romania.....377
52. **ORGANIC-MINERAL MODIFIER FOR PETRIFICATION OF WOOD**, N.V. Kiliusheva A.M. Ayzenshtadt V.E. Danilov A.A. Stenin, Northern Arctic Federal University named after M.V. Lomonosov Faculty of Civil Engineering and Architecture, Russia.....385
53. **PHASE TRANSITION OF HEXAGONAL BE NANOCRYSTAL INTO CUBIC SUPERLATTICE UNDER X-RAY RADIATION**, Mels Boranbayev, Gulmira Yar-Mukhamedova, PhD Farabi Bozheyev, Zhasulan Nakysbekov, Madi Aitzhanov, Al-Farabi Kazakh National University, Kazakhstan.....393
54. **POLYMER NANOCOMPOSITES OF POLYAMIDE/POLYETHYLENE/FUNCTIONALIZED CARBON FIBRES**, Alexandrescu Laurentia, Georgescu Mihai, Ficai Anton, Trusca Roxana, Tudoroiu Ligian, INCDTP-Div. Leather and Footwear Research Institute ICPI, Romania .....401
55. **PRODUCTION OF POLYMER CONCRETE COMPOSITIONS EFFECTIVE IN UNDERGROUND AGGRESSIVE WATERS**, Prof. Nikoloz Chikhradze, Prof. Guram Abashidze, M.Sc. Davit Tsverava, G. Tsulukidze Mining Institute, Georgia .....409
56. **PROPERTIES OF ANTI-CORROSIVE FERRITE PIGMENT SYNTHESIZED WITH THE USE OF PRODUCTION WASTE**, Sergey N. Stepin, Elvira I. Garifullina, Vladimir E. Katnov, Ilgiz V. Usmanov, Svetlana I. Tolstosheyeva, Kazan (Volga Region) Federal University, Russia .....417
57. **RESEARCH AND MATHEMATICAL MODELING OF THE PROCESS OF OBTAINING A NANOCOMPOSITE OF SiC-CNT**, Ms Anna Shaneva, Prof. Eleonora Koltsova, Assoc. Prof. Andrey Zhensa, Prof. Evgene Zharikov, Ms. Nelly Popova, Mendeleev University of Chemical Technology of Russia, Russia .....425
58. **RETENTION CAPACITY OF POLYSULFONE MEMBRANE IN WASTEWATER TREATMENT**, Laurentia Geanina TIRON, Eliza DANAILA, Gina Genoveva ISTRATE, Stefan BALTA, Maria VLAD, Dunarea de Jos University of Galati, Romania.....433
59. **STATISTICAL EVALUATION OF NUTRITIONAL CHARACTERISTICS FOR SEVERAL CHEESE TYPES**, Assoc. Prof. Dr. Ariana - Bianca Velcirov, Assist. Prof. Dr. Sofia Popescu, Lecturer Dr. Antoanela Cozma, Lecturer Dr. Dacian Lalescu, Assoc. Prof. Dr. Ing. Ioan David, Banat University of Agricultural Sciences and Veterinary Medicine King Michael I of Romania from Timisoara, Romania .....441
60. **STATISTICAL MODELING OF PHYSIC-CHEMICAL AND BIOCHEMICAL CHARACTERIZATION OF VARIOUS SMOOTHIE TYPES**, Assist. Prof. PhD Sofia Popescu, Assoc. Prof. PhD. Ariana Velcirov, Assoc. Prof. PhD. Alma Nicolin, Lecturer PhD Dacian Lalescu, Lecturer PhD Lia Micula, Banat University of Agronomical Sciences and Veterinary Medicine, Romania .....449
61. **STUDIES ON DANUBE WATER FILTRATION PERFORMANCE OF NANOCOMPOSITE ULTRAFILTRATION MEMBRANES**, Stefan Catalin PINTILIE, Marius BODOR, Andreea Liliana LAZAR, Iulian Gabriel BIRSAN, Stefan BALTA, University "Dunarea de Jos", Romania.....457
62. **SUPERCritical EQUIPMENT OF DIFFERENT VOLUME TO PRODUCE AEROGELS IN FORM OF PARTICLES - PROSPECTS OF SCALE-UP**, Menshutina N.V., Lovskaya D.D., Lebedev A.E., D. Mendeleev University of Chemical technology of Russia, Russia .....465
63. **SURFACES MORPHOLOGY, ROUGHNESS AND WETTING PROPERTIES OF NANOPOROUS ALUMINUM OXIDE FILM FORMED ON 1050 ALUMINUM ALLOY BY CONTROLLED ELECTROCHEMICAL OXIDATION**, V.M. Dumitrascu, L. Benea N.L. Simionescu, Dunarea de Jos University of Galati, Romania.....473
64. **TECHNOLOGICAL METHODS TO REDUCE WELDING STRESSES AND DISTORTIONS**, Corneliu Rontescu, Dumitru-Titi Cicic, Alexandru-Daniel Bucur, Ana-Maria Bogatu, University Politehnica of Bucharest, Romania .....481
65. **THE INFLUENCE OF THE WAY OF DEPOSITING THE FILLER MATERIAL ON THE GEOMETRICAL CHARACTERISTICS OF THE WELD BEAD**, Corneliu Rontescu, Dumitru-Titi Cicic, Ana-Maria Bogatu, Petriceanu Constantin, University Politehnica of Bucharest, Romania .....489

- [3] Grischenko L.A., Parshina L.N., Larina L.I., Trofimov B.A., Kanitskaya L.V., Novikova L.N. Propargylation of arabinogalactan with propargyl halides - a facile route to new functionalized biopolymers//Carbohydrate Research, England, vol.376, 2013, pp.7-14.
- [4] Makhotina L.G., Kuznetsov A.G., Akim E.L., Gerchin D.V., Ovchinnikova V.P., Potapova I.V. The use of biopolymer arabinogalactan as a plasticizing additive in concrete and mortars, Building materials, Russia, vol.12, 2012, pp. 4-6.
- [5] Fang, G.-Z., Ma, Y.-L., Xu, F.-Y., Huang, Z.-H. Study on ultrasonic extraction of arabinogalactan from wood Linchan Huaxue Yu Gongye, Chemistry and Industry of Forest Products, China, vol. 24, Issue 4, 2004, pp. 103-106.
- [6] G. Gröll , B. Forsthuber, M. Ecker. Sensitivity of waterborne coating materials to high acidity and high content of arabinogalactan in larch heartwood, Progress in Organic Coatings, USA, vol.101, 2016, pp. 367-378.
- [7] Babkin V.A., Ostroukhova L.A., Malkov Y.A. Biologically active substances from larch wood, Chemistry for sustainable development, vol 9, Russia, 2001, pp. 363-367.
- [8] Mucalo M.R., Bullen C.R., Manley-Harris M., McIntire T.M. Arabinogalactan from the Western larch tree: a new, purified and highly water-soluble polysaccharide-based protecting agent for maintaining precious metal nanoparticles in colloidal suspensions, Journal of Materials Sciences, Netherlands, vol.37, 2002, pp. 493-504.
- [9] G. Gröll , B. Forsthuber, M. Ecker. Sensitivity of waterborne coating materials to high acidity and high content of arabinogalactan in larch heartwood, Progress in Organic Coatings, USA, 2016, pp. 367-378.
- [10] Kuznetsov A.G., Makhotina L.G., Akim E.L., The use of the biopolymer arabinogalactan in the production of cellulose composite materials, Design. Materials. Technology, Russia, vol.5, 2012, pp. 82-84.
- [11] Koptyaeva E.I., Muhdarisova R.H., Kolbin A.M., Interaction of arabinogalactan of Siberian larch with chlorsulfuron, Journal of the Bashkir state University, Russia, vol.17, 2012, pp. 38-41.
- [12] Medvedeva E. N., Babkin V. A, Makarenko O.A., Obtaining high-purity larch arabinogalactan and investigation of its immunomodulatory properties, Chemistry of plant raw materials, Russia, vol.4, 2004, pp.17-23.
- [13] Veshnyakova L.A., Drozduk T.A., Ayzentadt A.M., Frolova M.A., Tutygin A.S., Surface activity of silicon-containing rocks, Materials science, Russia, vol.5, 2016, pp. 45-48
- [14] Veshnyakova L.A., Ayzentadt A.M., Frolova M.A., Estimation of surface activity of highly dispersed raw materials for composite building materials, Physics and chemistry of materials processing, Russia, vol.2, 2015, pp. 68-72.

## PHASE TRANSITION OF HEXAGONAL Be NANOCRYSTAL INTO CUBIC SUPERLATTICE UNDER X-RAY RADIATION

Associated Prof. Mels Boranbayev<sup>1</sup>

Prof. DrSc Gulmira Yar-Mukhamedova<sup>1</sup>

PhD Farabi Bozheyev<sup>2</sup>

Dr Zhasulan Nakysbekov<sup>1</sup>

Dr Madi Aitzhanov<sup>1</sup>

<sup>1</sup>Al-Farabi Kazakh National University, Kazakhstan

<sup>2</sup>National Research Tomsk Polytechnic University, Institute of High Technology Physics, Russia

### ABSTRACT

The structure and phase composition of annealed and irradiated beryllium plates were studied by X-ray analysis. Durable X-ray irradiation leads to phase transition of a normal hexagonal beryllium lattice into a beryllium superlattice. This superlattice is composed of beryllium superatoms that form a face-centered cubic lattice with the lattice parameter of 6.2205 Å and a superatom core that crystallizes into a diamond-type lattice with the lattice parameter of 1.5703 Å. It is shown that beryllium has three phase states: normal (hexagonal lattice), a superlattice which composed of nanocrystals beryllium and form F-structure, a nanocrystallites core which is composed of 56 atoms (the magic number) crystallizes in a diamond-type lattice. It was found that by doping with beryllium various alloys after heat treatment, it is relatively easy to form covalent bonds between the atoms of "Be" and alloys. This results in increased strength, hardness, elasticity, and corrosion resistance of the resulting materials (alloys). Good reflectivity of neutrons can be explained by a very high density and magnetic moment of superatom.

**Keywords:** nanocrystal, superlattice, x-ray radiation, beryllium, superatom

### INTRODUCTION

The prerequisites for our research were the results published by Russian scientists. Professor K.M. Yerokhin under the guidance of Academician Yu. E. Nesterikhin made model calculations for metal crystals in which they showed that with an electron deficit of 14%, the new phases are formed which should lead to the splitting of the main metal peaks [1, 2]. We first observed this effect in all metals from beryllium to tungsten under the irradiation of metals by high-energy electrons (3 MeV). A similar effect we found on beryllium when irradiated with X-rays.

It is known that for super atoms in 1987, chemists received the Nobel Prize, and Japanese scientists, when they studying nano-powders by mass spectroscopic methods, observed nano-clusters with magic numbers [3]. Since nano-clusters with magic numbers are more stable than others, then binding energy in these clusters should be higher. It means that the distance between atoms will be much smaller, which in turn leads to a decrease in parameters of quasi-cells. As for massive poly crystals, they consist of individual crystallites with dimensions of about  $10^{-8}$ - $10^{-7}$  m, there are fillers

from individual atoms, amorphous compounds  $10^{-10}$ - $10^{-8}$  m and fine crystallites  $10^{-9}$ - $10^{-8}$  m between them [4-5]. Consequently, we should observe our effects in massive samples.

Fundamental properties of nanosized structures like quantum dots and wells, quantum wires, clusters etc. were actively researched in the last decades with a view to create new materials with controlled mechanical, electrical, magnetic and optoelectronic properties, particularly for construction of new microelectronic devices. Formations from one to thousands of atoms attract interest among the microscopic objects clusters since they are in intermediate state between individual atoms and solid, and these formations show properties that are completely different from both of these states [6-9]. The understanding of how transition occurs from atoms to solid (including changes in their properties) opens way for getting fundamental knowledge as well as practical application.

Metallic clusters take a special place among various types of clusters as they have unique future due to their electronic structure and simplicity of their production [10], [11], [12]. In this respect beryllium becomes a strategic material that is widely used in practical human activity. Doping of steel, copper and other alloys with beryllium allows production of hard and corrosion resistive materials widely used in nuclear power plants as well as in producing materials for rocket and cosmic industries [13], [14], [15].

In this paper we report on a new phase of Be with the face-centered cubic superlattice that contains beryllium superatoms or clusters in the lattice nodes with the diamond-type lattice. We have done a systematic research of phase transition of beryllium treated by high temperature and X-ray irradiation into a Be superlattice.

## MATERIALS AND EXPERIMENTAL PROCEDURE

The material for the study was taken pure beryllium plate. Beryllium plates was studied without processing, after annealing, after 10 hours and after a long time (up to 100 hours) exposure with X-rays. The annealing procedure of pure beryllium plates was performed in an argon atmosphere at 1000 °C for 15 min. Irradiation of beryllium plate was performed by  $\text{CuK}\alpha$  radiation (1.5408 Å) for 10 h and for more than 100 h. The structure and phase composition of the plates were characterized by scanning electron microscope Quante 3D 200i and X-ray diffractometer DRON-7.

Sample's features. Microstructure and energy disperse X-ray analysis of beryllium samples presented in Table 1 shows the content of Be, C, O elements. Discrepancy of the content of elements in the table and intensity of peaks in the figure is explained by fact that beryllium is a very light metal, and diffraction pattern is created mainly from the inner electrons, beryllium has only two electrons, but carbon and oxygen have more inner electrons. Energy dispersive X-ray (EDX) analysis showed that initial beryllium plate consists mostly of beryllium and small amount of oxygen and carbon. X-ray patterns of initial, annealed and irradiated beryllium samples are shown in Figure 1. Beside characteristic beryllium peaks noted as H (hexagonal) there are also low angle peaks. These peaks are called superstructural because they correspond to the elementary unit cell with the bigger lattice parameter [12]. After treatment by high temperature and X-ray irradiation the intensities of the peaks change considerably, e.g., the cubic reflections as (110), (111), and for hexagonal - (111), (002), etc. In the Table 2

structure-sensitive peaks of three beryllium phases are reduced to one scale. After long X-ray irradiation treatment the content of Be superlattice is increased by two orders of magnitude. Our research strives to understand and explain this phenomenon.

Table 1 EDX analysis of pure beryllium plate

Element	Wt%	At%
BeK	89.99	92.72
CK	7.61	5.89
OK	2.40	1.39

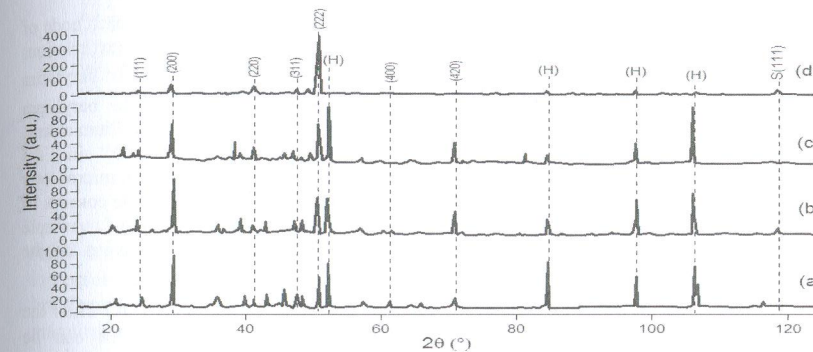


Figure 1. X-ray patterns of a) initial Be (sample 1), b) annealed (sample 2), c) irradiated during 10 hours (sample 3), and d) more than 100 hours (sample 4).

Table 2 Intensities of the peaks reduced to one scale

Be	Superlattice, a=6.2205 Å		Hexagonal (H)		Superatom core, a=1.55 Å
	(200)	(222)	(011)	(110)	(111)
Pure	0.255	0.140	0.226	0.193	-
Annealed	0.243	0.180	0.180	0.146	0.054
Irradiated, 10 h	0.405	0.300	0.155	0.111	0.012
Irradiated, more than 100 h	0.200	1.000	0.0081	0.081	0.138

The X-ray diffraction patterns shows superlattice reflections that correspond to a hexagonal loose packed (H) and cubic close packed lattices (F-lattice), see Fig. 2. The calculated parameters of the hexagonal unit cell are  $a = 5.0786$  Å and  $c = 10.77$  Å, and the parameter of the unit cell of the face-centered cubic lattice (F-lattice) is 6.2205 Å. This cubic cell fits into the hexagonal

cell, see Fig. 2a. It should be noted that the parameter of the superlattice exceeds the standard value of the beryllium lattice.

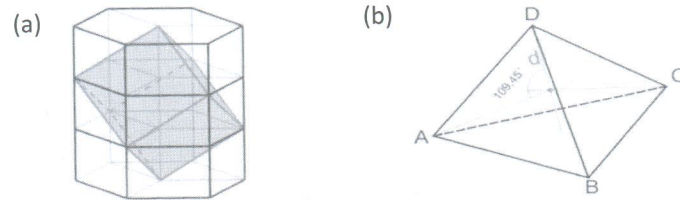


Figure 2. A cubic superlattice presented in hexagonal lattice (a) and a diamond-type lattice (b)

Therefore clusters (nanoparticles) larger than beryllium atom should be (seated) at each node of the superlattice. The radius of such cluster (nanoparticle) was determined from the next relation:  $R = a / \sqrt{4} = 2.199 \text{ \AA}$ . The calculated value of the radius is greater than the radius of beryllium atom (1.43 \text{ \AA}). Comparing the radius of beryllium atom and the radius of the beryllium nanoparticle we can make a conclusion that the nanoparticle cannot consist of beryllium atoms. It is possible that Be is associated in doubly ionized state in the nanoparticle as  $\text{Be}^{2+}$  since the primary oxidation level of Be is +2 and Be ion radius is 0.34 \text{ \AA}. Based on electron microscopy data on homogeneous composition of the sample, we assumed that the nanoparticle consists of beryllium ions and sp-hybridization of Be-Be binding levels results in formation of quadruple covalent  $\sigma$ -bonding between the ions. Such bonding should cause crystallization of the beryllium ions into a diamond-type lattice.

Based on this assumption the distance  $d$  between atoms of Be-Be is 0.68 \text{ \AA}. Then the lattice parameter of the unit cell of the crystal inside the nanoparticles can be determined from the following relationship:  $a = 4d / \sqrt{3} = 1.5703 \text{ \AA}$ . Thus, the X-ray patterns must have the traces of three phases of Be: hexagonal, face-centered cubic superlattice, and superatom core crystallized into the diamond-type lattice. Two phases of Be are present in all X-ray patterns (Fig. 1 a, b, c, d). Calculations showed that on copper  $\text{CuK}\alpha$ -radiation only one peak should be present on X-ray pattern (111) corresponding to the nanocrystallite (superatom). Other peaks corresponding to (220), (222) and (400), etc. are outside of the restriction sphere due to the small size of the unit cell parameter. According to calculations the diffraction peak from the nanocrystallite should be located at an angle of 116.33°. Such peak is detected at the irradiated and annealed diffractograms, but it does not exceed the background level on the diffraction pattern of initial Be. Experimental value of the angle of the diffraction peak of annealed sample is 118.48°, and of irradiated sample it is 118.40°. Calculation of the parameter from the experimentally detected angle gives the value of 1.5514 \text{ \AA} representing a deviation of more than 2°, and the intensities of these peaks vary greatly as per the data shown in the Table 1. It should be noted that irradiated sample (Fig. 1d) differs substantially from the initial and annealed beryllium.

In order to detect reflections from outside of the restriction sphere we irradiated sample corresponding to Fig. 1d by  $\text{MoK}\alpha$  (0.70926 \text{ \AA}). In Fig. 3 the X-ray patterns show that along with the (111) reflection there are additional diffraction peaks corresponding to (220), (222) and (400), which prove the presence of superatom structure. These diffraction peaks fall within the restriction sphere due to larger value of  $\text{MoK}\alpha$  wave vector in comparison to  $\text{CuK}\alpha$ . The calculated lattice parameter of the superatom core is

1.547 \text{ \AA} that is matched with the presupposed lattice parameter 1.5703 \text{ \AA}. The calculated ionic radius of the superatom core is 0.3349 \text{ \AA}, which is less than doubly ionized state of Be.

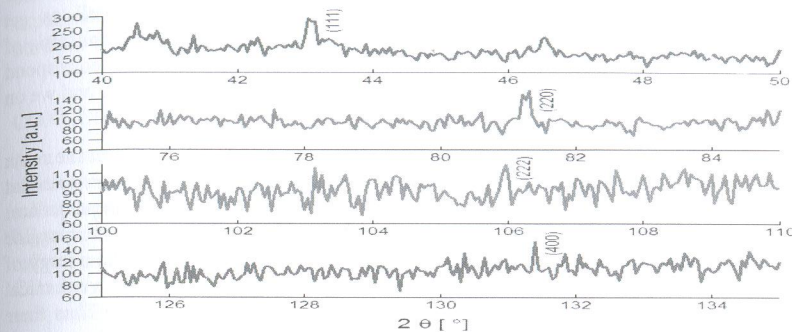


Figure 3. The X-ray pattern of Be plate irradiated more than 100 hours at different ranges

After irradiation the (222) diffraction peak of the cubic superlattice dramatically increases compared to the values of other considered peaks. Background of X-ray irradiated beryllium is decreased; the content of beryllium is by two orders of magnitude less than in pure beryllium. The structure of beryllium superlattice after irradiation is quantitatively increased and improved approaching monocrystalline state since the background on monocrystals is much. The difference between the calculated and experimental values of the parameter is 0.02 \text{ \AA} (or about 1%), which can be considered as a good match. Average measurement accuracy of diffractometer is 0.01%. The mechanism of the beryllium regeneration after annealing can be explained as follows: annealing at 1000°C in argon environment leads to fragmentation of micro-crystallites of the polycrystalline sample to nano-crystalline state because of hybridization of Be atoms. In turn the fragmentation occurs as follows: at hybridization interatomic distance of Be-Be atoms drastically reduces and there appears significant strain between excited and non-excited regions, and when the strain exceeds the interatomic interaction the crystal breaks in full or in part. Fragmentation continues while the energy of the external impact does not exceed the binding energy of nanocrystallite atoms. However nanocrystal clusters of atoms less than 2.199 \text{ \AA} agglomerate to the optimal value of 2.199 \text{ \AA} because of sp-hybridization and formation of Be-Be bonding. Thus, the dielectric nanocrystallite with a certain number of atoms (the magic number) that behaves as a single atom of the periodic table is formed (beryllium model) [13], [14]. Since shared electrons (electrons of loosened level) are located at the orbitals around nanocrystallite (superatom core) forming an "electronic cloud", each nanocrystal can be called superatom. Such superatom has a nucleus consisting of 56 atoms of beryllium with the electrons concentrated on the surface. Around the nucleus there are electron orbitals with an even number of electrons ("electron cloud"), because of that a dipole-dipole interaction similar to the interaction



between the atoms of inert gases occurs between superatoms resulting in crystallization and formation of F-lattice. But the process of hybridization does not proceed effectively at high temperatures (the annealing temperature) although structurally sensitive (222) reflection of F-lattice is increased (Fig. 4). However the effect is not obtained after irradiation. Apparently this is due to the fact that there reverse processes occur after annealing, i.e. particles less than superatom in size agglomerate as well as get destructed. Therefore we assume that durable annealing should lead to establishing of equilibrium. From the calculated data, all the peaks of the roentgenograms correspond to beryllium, whatever phase they were  $\alpha$ - or  $\beta$ - are located further than  $25^\circ$ , and we on the X-ray patterns observe peaks of  $2\theta$  from  $10^\circ$  to  $20^\circ$ .

This process becomes much more active when Be is irradiated with X-rays at the room temperature. The mechanism of superatom formation during irradiation is somewhat different. Formation of superatom during irradiation occurs in the following sequence: electrons ejected by X-rays (photoelectric effect) leave the crystallite (dielectric) resulting in it being positively charged up to the point where the energy of the Coulomb repulsion exceeds the binding energy leading to significant mechanical stresses in the crystallite that break the crystal ("Coulomb explosion" [1]). Thus there occurs a process of radiation crushing up to nano-size. The process continues until stable nanocrystals that we call superatoms are formed. Apparently the formation of superatoms can occur in two ways:

a) Crushing makes the size of large quantity of nanocrystals smaller than the superatom  $R_{at} = 2.199\text{\AA}$  (atoms of which are excited). Further, these nanocrystals are closing in leading to their agglomeration and hybridization on binding levels which in turn leads to formation of covalent  $\sigma$ -bonding (Pauli Exclusion Principle);

b) the electronic structure of nanocrystals with dimensions equal to  $R_{at}$ , change at the expense of the inner electrons of the nanocrystallite leading to formation of covalent  $\sigma$ -bonding within the nanocrystallite, while free electrons (at the loosed level or in conduction band) migrate to the orbit around nanocrystallite (superatom core).

Both processes lead to the formation of nanocrystallites (superatoms): the "top-down" process arising from radiation crushing, and "bottom-up" process where smaller smaller clusters of atoms and nanocrystallites agglomerate.

Table 3 Density of the different phases of beryllium

Lattice type	a, $\text{\AA}$	c, $\text{\AA}$	$\rho$ , g/cm <sup>3</sup>
Table value	2.2860	3.584	1.848
FCC superlattice	6.2205	-	3.538
Hexagonal superlattice	5.0786	10.77	3.538
Nanocrystallite	-	-	21.00
Superatom core (diamond lattice)	1.5514	-	32.008

The next step was to determine the number of Be atoms in the superatom core, the superatom structure and density. The number of atoms of Be in the superatom core was calculated using the analytical and geometric (5th coordination sphere) methods. The calculated values showed that the superatom contains 56 atoms (ions) of Be. Since the

structure and electronic structure of three Be phases are different, the densities are also different for each phase. The calculated values of the density of the samples are listed in Table 3. Comparative analysis of the data shows that the density of three phases of beryllium significantly differs. The most significant difference is observed between the density of (nanocrystallite) superatom and superatom core. This serves as an experimental confirmation of the formation of superatom with "electron cloud" and covalent  $\sigma$ -bonding of Be-Be.

## CONCLUSIONS

As a result of the indexing diffractograms of annealed and irradiated beryllium besides characteristic lines of the metal, there are lines in the lower angles. These lines were called superlattice lines, because it was found that they belong to the unit cells with bigger parameters. The results of the calculations showed that the superstructure reflections can be represented as a hexagonal close packed and cubic close packed. Calculated parameters of the hexagonal unit cell are  $a = 5.0786\text{\AA}$ ,  $c = 10.77\text{\AA}$ , and the unit cell parameter of F-cubic lattice  $a = 6.2205\text{\AA}$ , thus the cubic cell fits into the hexagonal unit cell. It should be noted that the parameters of superlattices have more parameters than table parameters of beryllium. Calculations showed that the sites of the superlattice of beryllium superatom has a radius of  $2.199\text{\AA}$ . The results of geometric (5th coordination sphere) and analytical methods have shown that beryllium superatom consists of 56 atoms (ions) of Be.

Thus, the confirmation of superatom formation is crystallization of beryllium into superlattice with the lattice parameter of  $6.2205\text{\AA}$ . We can make a conclusion that our assumptions were correct. The results of this work lead us to believe that doping of various alloys with beryllium and consequent treatment with high temperature enables relatively easy formation of covalent bindings between the atoms of Be and alloys, which in turn increases strength, hardness, elasticity and corrosion resistance of the treated materials (alloys). Good reflectivity of neutrons can be explained by very high density and magnetic moment of superatom.

## ACKNOWLEDGMENTS

This work was supported by al-Farabi Kazakh National University, Institute of Experimental & Theoretical Physics by AP05130069 project "Development of nanotechnology for the synthesis of functional galvanic coatings for electrical equipment components."

## REFERENCES

- [1] Yerokhin K. M., Kalashnikov N. P., Nesterikhin Yu. Ye., Ol'chak A. S. Kulonovskij vzryv shchelochnyh i perekhodnyh metallov pri chastichnom udaleni ehlektronov provodimosti. Dokl. Akad. Nauk, vol.436/ issue 4, pp 464-469, 2011.
- [2] Mukul K., Mookerjee A., Bhattacharya A. Structure and stability of copper clusters: A tight-binding molecular dynamics study. Phys review. A 69, 043203, 2004.
- [3] Poole Ch.P., Owens F.J. Introduction to nanotechnology. 336 p. 2003.

- [4] Ved' M., Sakhnenko N., Nenastina T. et al. Electrodeposition and properties of binary and ternary cobalt alloys with molybdenum and tungsten // *Appl. Surf. Sci.*, vol. 445, pp 298-307. 2018.
- [5] Yu.A. Baykov, V.M. Kuznetsov. Fizika kondensirovannogo sostoyaniya. M.: Binom. Laboratoriya znaniy, 293 p. 2013.
- [6] Pavlov P.V., Khokhlov A.F.. Fizika tverdogo tela. – M.: Lenand, 2015.– 496 p.
- [7] Muradov, A., Mukashev, K. et al. Impact of silver metallization and electron irradiation on the mechanical deformation of polyimide films // *Technical Physics*, vol. 62 / issue 11, pp 1692-1697, 2017.
- [8] Mussabek, G., Sagyndykov, A. et al. Modern state of composite coatings formation problem // 17th Int.I Multidisc. Sc Geoconf. SGEM 2017. 17 (61), 2017, Pp 233-240. 130800Fan.
- [9] Muradov, A., Mukashev, K. et al. Mathematical model of composite materials formation // 17th Int.I Multidisc. Sc Geoconf. SGEM 2017. 17 (61), 2017, Pp 201-208. 130800
- [10] Ved' M., Sakhnenko N., Karakurkchi A., Yermolenko I. *Appl. Surf. Sci.*, vol. 383, pp 346–352. 2016.
- [11] Darisheva A., Kasimzhanov K. et al. Physicochemical Investigations of Scheelite Concentrate Decomposition // *Euras. Chem.-Technol. J.*, № 17, p. 209–212, 2015.
- [12] Ivanov V.K., Ipatov A.N. Ed. J.-P. Connerade. Singapore: World Sci., vol.141, 2006.
- [13] Ved' M., Sakhnenko N., Koziar M. et al. Ternary cobalt-molybdenum-zirconium coatings for alternative energies // *Appl. Surf. Sci.*, vol. 421. pp 68-76, 2017.
- [14] Yar-Mukhamedova, G.Sh., Sakhnenko, N.D., Ved, M.V. Surface analysis of Fe-Co-Mo electrolytic coatings // *IOP Conference Series: Materials Science and Engineering*. 213 (1) 012019
- [15] Sagyndykov, A.B., Kalkozova, Zh.K. et al. Fabrication of nanostructured silicon surface using selective chemical etching // *Technical Physics*, vol.62/ issue 11, pp 1675-1678, 2017.

## POLYMER NANOCOMPOSITES OF POLYAMIDE/POLYETHYLENE/ FUNCTIONALIZED CARBON FIBRES

**Dr. ALEXANDRESCU LAURENTIA<sup>1</sup>**

**Ing. GEORGESCU MIHAI<sup>1</sup>**

**Assoc. Prof. Dr. FICAI ANTON<sup>2</sup>**

**Dr. TRUSCA ROXANA<sup>2</sup>**

**Phs. TUDOROIU LIGIAN<sup>3</sup>**

<sup>1</sup> National Research And Development Institute For Textile And Leather - Division Leather And Footwear Research Institute **ROMANIA**– INCDTP-ICPI;

<sup>2</sup> Faculty Of Applied Chemistry And Materials Science, University POLITEHNICA Of Bucharest **ROMANIA**;

<sup>3</sup> SC RONERA SA **ROMANIA**

### ABSTRACT

In this paper, combined effects of carbon fibres treatment and compatibilizer polymers (PE-g-MA) on the structure and properties of PA/PE/PE-g-MA/ functionalized carbon fibres composites were studied. The optimum formulation was used to prepare a series of nanocomposites under different technological conditions. Also, a correlation between their physico-mechanical properties and IR spectra (ATR technique) was proposed.

The carbon fibres functionalisation consisted in oxidizing the nanoparticles with oxidant mixture of  $K_2Cr_2O_7/H_2SO_4$ . The carbon fibers were immersed in the oxidant mixture at 60°C for 2h - followed by washing, drying and control.

The nanocomposites based on PA/PE-g-MA/PE/functionalized carbon fibres were characterized by scanning electron microscopy (SEM), Fourier transform infrared spectrum (FT-IR), and physico-mechanical tests.

**Keywords:** nanocomposites, polyamide, polyethylene, compatibilization agent, functionalized carbon fibres.

### INTRODUCTION

Compounding polymers are widely used to obtain new materials. The disadvantage is that the polymers are usually not compatible and the preparation of compounds with suitable (mainly processing and physico-mechanical) properties is not performant. Polyamide (PA) is a thermoplastic material, widely used in the industry, with varied applications (e.g. fibres, films, textiles, and various casting products) due to its mechanical and thermal properties. However, it has some limitations, such as: humidity absorption, sensitivity to shock, relatively low impact resistance and a weak dimensional stability. As a result, it is necessary to modify PA to improve physical-mechanical properties favourable for the industrial environment [1-4]. Polyethylene is a thermoplastic polymer obtained by polymerizing ethylene at low, medium or high pressures, with the use of oxygen as initiator. It is presented in translucent solid form