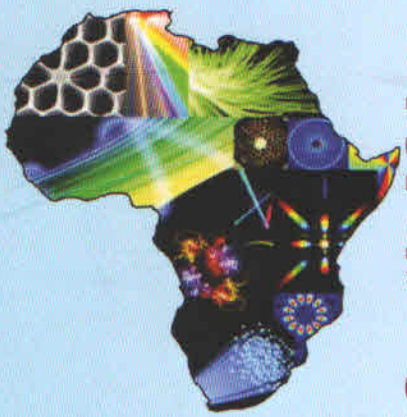

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45 - The capture cross sections at the electron collisions with hydrogen atom and proton in the dense semiclassical plasma

Poster Session - Monday 11 July 2016 16:51

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Investigation of the interaction between particles and plasma properties is of great interest in many areas of physics such as atomic and plasma physics. It is important for the development of the plasma technologies. One of the elementary processes in plasma is the electron capture process. In this work the electron capture processes by the hydrogen atom and proton were investigated. The motion of the electron in the field of the the motionless atom or proton was considered on the basis of the perturbation theory and the solving of the equation of motion. The interaction potentials between the electron and the hydrogen atom and also proton were presented in works [1,2]. These effective potentials, taking into account the quantum-mechanical effects of diffraction of particles and plasma screening effects, have finite values at the distances close to zero.In this work the electron capture radius, which was determined by equating the kinetic energy of impacting electron and the interaction energy between the electron and the hydrogen atom or proton, was presented. The trajectories of the electron in the field of the atom and proton were simulated. Obtained results of the electron capture by the atom and proton were compared. Using the electron capture probability, the electron capture cross section was calculated. References[1] T.S. Ramazanov, K.N. Dzhumagulova, Effective screened potentials of strongly coupled semiclassical plasma, Phys.Plasm. 9 (2002) 3758-3761[2] T.S. Ramazanov, K.N. Dzhumagulova, Y.A. Omarbakiyeva, Effective polarization interaction potential "charge-atom" for partially ionized dense plasma, Phys. Plasm. 12 (2005) 092702

46 - Multiscale simulations of structure and thermomechanical properties of phthalonitrile heat-resistance resins

Poster Session - Monday 11 July 2016 17:12

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Phtalonitrile-based matrixes are thermostable resins used for durable reinforcement materials. The resins are typically produced by two-stage curing of phthalonitrile monomers in presence of initiator. During the first low temperature stage (~200°C), nitrile groups transform into inter-monomer bonds between isoindoline groups, which is the typical polymerization path. The second curing stage is aimed to reach higher conversion rate and produced at elevated temperatures (300 – 350°C), at which triazine can be formed by three monomers. Effectively, triazine is a triple link between monomers, making the topology of the polymer network even more complex. The effect of triazine crosslinks in the structure and physical properties of the material is important but unclear up to now.We have developed a multiscale simulations scheme of phthalonitrile thermosetting resins. The scheme contains a set of consecutive phases from dissipative particle dynamics (DPD) level to molecular dynamics. On the first step, we simulate two-stage curing process with DPD technique. The length of low-temperature and high-temperature stages is controlled by the aim conversion rates known from experimental study. On the next step, a reverse mapping procedure is used to convert coarse-grained structures onto atomistic ones. The obtained atomistic structures are then refined by a Monte Carlo procedure with soft repulsive potentials to avoid insufficient structural motifs such as the short cycle spearing. Then we run short relaxation within molecular dynamics (MD). The prepared material samples are used for the following MD simulations to estimate thermophysical and mechanical properties of the material. In this report, we present and discuss thermophysical and mechanical properties for the phthalonitrile matrixes obtained with using different comonomers and polymerization protocols.

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