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NANO- POROSITY FORMATION COMPUTER SIMULATION *)

Zmievskaya G.I.

Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, Moscow, Russia, zmig@mail.ru

The successful implementation of the computational experiment in plasma was the creation of kinetic codes for solving problems of collisionless highly nonequilibrium plasma [1]. Kinetic models of the nonequilibrium phase transition (PT) stage (nucleation) of the formation of vacancy-gas porosity in thin layers of the "metal-dielectric" surface during implantation of inert gas ions, which changes the mechanical, electrical, optical and thermophysical properties of materials when filling the porosity with various substances, including those having a large the refractive index, thus there is a prospect for changes in the optical properties of the material. Models of porous media can be used to change the coefficient of thermal conductivity in controlled combustion problems, as well as for blistering in diagnostic mirrors, plasma treatment of surfaces with a porous capillary structure, etc. Gorenje computer simulation/CS/ is understood as the calculation on a computer of an analog of the studied physical process, CS allows you to study phenomena in those conditions where the fields of application of the theory end, or "can serve as the basis for new theories" [1].

The nucleation problem of the phase transition/PT/of the 1st kind of PT, known as the Vollmer-Becker-Doering-Frenkel-Zeldovich problem [2] has been modified for non-stationary cases with the solution of quasi-linear Fokker-Planck-Kolmogorov type equations /FPK/, taking into account the long-range oscillating interaction potential of clusters of PT nuclei in a solid by the method of stochastic molecular dynamics /SMD/ based on the solution of stochastic Ito-Stratonovich equations /SDE/ [3,4] by a numerical method with second-order root-mean-square convergence and algorithms with an infinite stability domain for SDE with additive noise, constructed for probabilistic measures that depend on the phase variables (here) : the clusters sizes of PT's nuclei, i.e. pores, and their centers of mass coordinates in a crystal lattice. As an example of the CS model of PT's nucleation: in the layers of the Mo/Si sample, under the action of Xe ++ ions with an energy of 5 keV in 10 -4 seconds, with a normal flux drop (10 15 -10 17 ions/cm 2), chains of pores up to 35 nm long can form parallel to the flux, depending on its fluence and surface temperature.

SMD research programs for solving quasi-linear FPKequations [3,4] can be part of hybrid codes in which plasma codes are supplemented by calculations of pores formation processes.

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