Nonequilibrium PHASE TRANSITIONS IN NANODISPERSED MEDIA: PATTERNS AND APPLICATIONS [[1]](#footnote-1)\*)

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Stochastic molecular dynamics of plasmochemical collisions [1] and dispersed media [2, 3] is consistent with plasma codes. Previously, kinetic plasma codes [4] made it possible to create a dust plasma code for a thermonuclear reactor divertor.

Phase transitions (PT) of the 1st kind at the initial nonequilibrium stage, when PT nuclei are formed (discharge plasma droplets or islands of the liquid/crystal phase of condensation on the surface) are called nucleation. When exposed to streams of inert gas ions on the sample, non-point vacancy-gas defects (VGD) are formed in the crystal lattice, PT occurs. The sizes of the PT nuclei and their distribution in the sample volume are determined by solving quasi-linear kinetic partial differential equations of Fokker-Planck with nonlinear coefficients (Kolmogorov-Feller, Smolukhovsky) and equations of the stochastic analogue of Ito in the. sense of Stratonovich by stable Rosenbrock scheme of the Monte Carlo methods family.

PT nucleation is represented by a superposition of two Brownian motion (BM) processes: diffusion in the phase space of nuclei sizes (or their clustering) and diffusion in Cartesian coordinates of the model volume, i.e., a model of a Brownian particle with variable mass. Fluctuations in the size of clusters of PT nuclei, both condensation droplets in the discharge plasma and VGD in a solid, depend on the model of Gibbs energy as the sum of the contributions of the nucleation energies, which makes it possible to calculate the probability density of the size distribution of clusters at volume points. Brownian motion of VGD clusters (in the case of ion implantation) is initiated by indirect elastic interaction between VGD and sample boundaries. The occurrence of VGD perturbs the oscillations of the acoustic phonons of the lattice, the frequencies of which change when scattering on defects, which is taken into account when deducing the dependence of the interaction potential on the coordinates of VGD in the volume and the elastic modulus of the medium [5]. Brownian diffusion in the calculations of BM in metals and semiconductors also depends on Friedel oscillations of the electron density. In the process of calculating the BM trajectories, the VGD interaction potentials are taken into account in a self-consistent manner when calculating the trajectories of stochastic molecular dynamics.

Computational experiments on the porosity of a nanodispersed medium can be used in sensor models and laser semiconductor plasma antennas, as well as in plasma treatment of surfaces with a porous-capillary structure. Numerical estimation of the rate of change in pore sizes and the distribution of local elastic stresses created by nanopores is of interest for controlling the properties of porous semiconductors, for creating dielectrics matrices with inclusions of metal nanoparticles in the interests of plasmonics. By varying the parameters of ion implantation (duration and intensity of flux, area and direction of exposure, surface temperature), it is possible to control the dispersity of media within a wide range.

References

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1. \*) [abstracts of this report in Russian](http://www.fpl.gpi.ru/Zvenigorod/L/Pt/ru/GA-Zmievskaya.docx) [↑](#footnote-ref-1)