Radiation damage thin coating of silicon carbid

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General physical and physico-chemical problems of ion implantation and radiation physics of solid body related with physical problems of inert gases ions implantation in crystal lattice are considered in computer experiments. This models are focused on research of radiation-thermal modification of properties of materials. Kinetic equations of Kolmogorov–Feller and Einstein–Smoluchowski had been formulated in general. The radiation damaging are able to be described in terms of probability density of distribution defects into lattice and this approach is applied to description of initial stage of first-order phase transition. The equations in partial derivative are solved using Stochastic Simulation Method /SSM/(original method which is similar to molecular dynamics but different from the approach of imitation real particles of lattice). We have used set of stochastic differential equations equivalent to kinetic equations in partial derivatives. Gaseous defects (pores) appear as a result of penetration into lattice of inert gas ions of high energy (about several keV). This model is used for prediction of radiation damage (in case of cover silicon carbide). The same model is considered for creation of new materials using radiation stimulated structures of porosity. Method of stochastic analogue[1] is based on theory according to which the kinetic equations of parabolic type are uniquely linked with stochastic differential equations /SDE/ Ito and with the density of transition probabilities of Markov random process, the solution of SDE's Ito can be interpreted as the distribution function /DF/of the corresponding kinetic equation[1, 3-5]. Coefficients of the kinetic equations depend on probability density defects distribution namely the thermodynamic potential of nucleation[3,4] (or Gibbs energy) and long-range potentials of indirect elastic interaction of lattice defects each with other (occurs through the perturbation of acoustic phonons lattice defects and Friedel oscillations of electrons density). Diffusion in the phase space of defects sizes {G} and diffusion in phase space {R} of crystalline lattices are accounted also as coefficients depended on DF. So, Brownian motion of radiation defects in thin layers of silicon carbide occurs under the influence of long-range forces. Stable solution of linear SDE's Ito-Stratonovich [2] is modified on a case quasilinear equations of model as stable numerical method the second order of accuracy with infinite area of sustainability (according to the new definitions and theorems of [2]) on a regular grid of time (without the limitations on the time step). Calculations have shown, that the porosity formation in a layer of silicon carbide depends on its thickness, doses, temperature and degree of discrepancy of parameters lattices layer of the coating and the substrate. Elastic stress from defects in the layers of mkm- thickness can reach value of stress corresponding discrepancy between lattice parameters of layers «coating-substrate» during of initial stage of nucleation (~ms). Study of the mechanisms of phase transition which are non-equilibrium at short time (about 10 mks) carry out by meance SSM. Calculations are important in fusion reactor materials science, electrical propulsion engines of the spacecraft, and also in the creation of porous semiconducting and dielectric materials [7].

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