POROSITY OF THE NANOSTRUCTURED THIN SILICON CARBIDE LAYER: COMPUTER SIMULATIONS OF THE BROWNIAN MOTION OF THE DEFECTS

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Porous semiconductor materials belong to the nanostructured media, the sizes of a pores and a crystal part of a sample are up to hundreds of nanometers from units, and the wide range of porosity in materials creates not only various dispersity, but also optical, luminescent and electric properties that assumes their use in solar batteries, photodetectors, light-emitting diodes, photon crystals, electroluminescent displays, thermoinsulators, waveguides and also any sensors, gas analyzers, sensors. Properties of porous silicon carbide, SiC, and methods of creation of porosity are relevant including means of a computing experiment [1] - modeling of the plasmas-like crystal media with not-point radiation defects (pores) which formation and Brownian motion are defined by elastic properties of a lattice (including oscillations of acoustic phonons). At a temperature of 900 K implantation of a stream of ions of Xe++ with energy ~5 keV was modelled, time of radiation is determined by a dose ~ 1016 cm–2, the percolation analysis of distribution of pores has allowed to estimate the sizes of precracks ~40–60 nanometers and the stretching tension in an order lattice   
1015 GPa, degree of dispersity of the sample depending on conditions of numerical experiments and flicker-noise ranges is defined. Conditions of creation of structures of porosity have been considered in model of Brownian motion of defects as stochastic system - the generator Van der Pol in the conditions of autogeneration [2]. The behavior of 2D model is studied by means of the kinetic equation of Fokker–Planck–Kolmogorov for density of transitional probability (kinetic function of distribution of f(x,V,t) where x is the coordinate, V is the rate, t is the time) and a stochastic analog of model – the stochastic differential equations of Langevin. Diagnostics of f(x,V,t)is given, and her visualization for various modes of the generator Van der Pol at variation of intensity of noise. The model allows to compare a condition of phase space of stochastic variables at change of a ratio of physical quantities which in model characterize phase transition: α, β, γ, are the coefficients of feedback, linear and nonlinear friction respectively.

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References

1. G.I. Zmievskaya, T.A. Averina, and A.L. Bondareva. Numerical solution of stochastic differential equations in the sense of Stratonovich in an amorphization crystal lattice model. Applied Numerical Mathematics,15–29, 2015.
2. Yu.L. Klimontovich. Statistical Theory of Open Systems. Dodrecht: Kluwer Acad, Publ., 1995.