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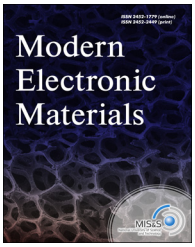

Mathematical modeling of point defect cluster formation in silicon based on molecular dynamic approach ☆

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Abstract
A very important task on the way of improving the technologies of synthesizing highly effective light-emitting diodes on the basis of silicon is theoretical research into the formation of point defect clusters. One method of obtaining silicon with photoluminescent properties is radiation impact. It causes the formation of various defects in its structure, including point and linear defects, their clusters and complexes. In this paper a mathematical model was used to determine the coordinates and velocities of all particles in the system. The model was used for describing point defect formation processes and studying their evolution with time and temperature. The multi-parametrical Tersoff potential was used for the description of interactions between particles. The values of the Tersoff potential were selected by solving the parametric identification problem for silicon. For developing the models we used the system cohesive energy values obtained by an ab initio calculation based on the density functional theory (DFT). The resultant computer model allows MD simulation of silicon crystal structure with point defects and their cluster with possible visualization and animation of simulation results.

Introduction

The mechanism of point defect cluster change and development into elongated {113} defects is one of the most important and understudied problems arising in the course of ion implantation of heavy metals in crystal silicon. Up to

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date, experimental data on possible types of point defect clusters in silicon have been obtained [1-3]. Besides, a great number of theoretical studies regarding their stability, evolution with time and in case of temperature variations have been conducted. Various approaches have been used. For example, theoretical researches [4,5] of point defects in silicon including calculations of the formation energy were performed using the first-principles (ab initio) calculations based on the density functional theory (DFT) [6,7]. In a earlier work [8], the migration process of point defects in silicon was considered using the *tight-binding molecular dynamics (TBMD) simulation method*. Papers [9,10] present the results of an experimental research using the high-resolution transmission electron microscopy (TEM) of complex self-organized defect structures formed in crystal silicon in the course of ion implantation of Er atoms with an energy of 2 MeV at 600 °C. Based on the TEM data and calculations with use of the HyperChem software package, it was demonstrated [9,10] that the said defect structures are essentially an aggregation of two split interstitial atoms and a divacancy that form a chain in the {113} plane. As far back as in 1964, possible existence of such defects was predicted by Watkins [11]. However, the first direct observation of such an ordered structure of defect complexes was only described much later [9,10]. The theoretical research of causes leading to the formation of complex defect structures-point defect clusters in silicon-and their evolution in time is a challenging and crucial task. Presented below is one of the possible approaches to looking for a solution along with the results of mathematical modeling of point defect clusters in silicon. The molecular dynamics (MD) simulation of point defect clusters in silicon was carried out using the multi-parametrical Tersoff potential. The perfect silicon structure along with silicon structures having various point defects was simulated.

Simulation of point defect clusters in silicon

For calculating the ordered cluster configurations of vacancies and interstitial atoms, we used multi-scale computerized modeling, where calculations at each scale level were performed using the respective computational models, techniques and approximations. The atomic-crystal and electronic structure of silicon with defects was simulated by means of the first-principle calculations based on the density functional theory using the plane wave basis and PAW-potentials (VASP software package) [12]. During the first-principles simulation of the perfect (defect-free) silicon structure, we used a periodic cell consisting of 64 atoms ($2 \times 2 \times 2$). The first-principle calculations were carried out using the supercomputers (computational clusters) of the Interdepartmental Supercomputer Center of the Russian Academy of Sciences and computer resources of the Lomonosov Moscow State University.

The changes in the defect structures and structures with defect clusters with time were simulated with the use of hybrid algorithms comprising the molecular dynamics methods and optimization methods [13] that allowed the selection of optimum values for interatomic potential parameters. In so doing, the results of the first-principle calculations were considered as reference ones. As an interatomic interaction potential for silicon, use was made of the many-body Tersoff potential [14] that demonstrated good results for the simulation of covalent compounds. Within the Tersoff method, the system cohesive energy (E) is described as follows:

$$E = \sum_i E_i = \frac{1}{2}\sum_i V_{ij}; \tag{1}$$

$$V_{ij} = f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right]; \tag{2}$$

$$f_R(r_{ij}) = A_{ij}\exp\left[-\kappa_{ij}\left(r_{ij} - R_e\right)\right]; \tag{3}$$

$$f_A(r_{ij}) = B_{ij}\exp\left[-\mu_{ij}\left(r_{ij} - R_e\right)\right]; \tag{4}$$

$$f_C(r_{ij}) = \begin{cases} 1, & r_{ij} < R - R_{cut}; \\ \frac{1}{2}\left[1 + \cos\left(\frac{\pi(r_{ij}-R)}{2R_{cut}}\right)\right], & R - R_{cut} < r_{ij} < R + R_{cut}; \\ 0, & r_{ij} > R + R_{cut}. \end{cases} \tag{5}$$

Here, r_{ij} are the distances between atoms with numbers i and j, respectively; A_{ij} and k_{ij} are the repulsion function coefficients; b_{ij}, B_{ij}, and μ_{ij} are the attraction function coefficients. For single-component silicon, the Tersoff potential comprises 12 parameters being specific for the substance simulated: D_e, R_e, β, S, n, γ, λ, c, d, h, R, R_{cut}. In this case, the R and R_{cut} parameters are determined from the experimentally that obtained geometrical characteristics of the substance and therefore require no selection.

For parametric identification of the Tersoff potential for silicon, we consider the following objective function:

$$\begin{aligned} F(\xi) = {} & \omega_1\left(E_{coh}(\xi) - E_{coh}^{fpc}\right)^2 + \omega_2\left(a(\xi) - a^{fpc}\right)^2 + \omega_3\left(B(\xi) - B^{fpc}\right)^2 \\ & + \omega_4\left(C'(\xi) - C'^{fpc}\right)^2 + \omega_5\left(C_{44}(\xi) - C_{44}^{fpc}\right)^2 \\ & + \omega_6\left(\zeta(\xi) - \zeta^{fpc}\right)^2 \to \min, \xi = (\xi_1, \ldots, \xi_m), \end{aligned} \tag{6}$$

Where E_{coh} is the cohesive energy, depending on Tersoff potential parameters; $a(\xi)$ is the lattice constant, which also depends on the potential parameters; $B(\xi)$ is the volume elasticity modulus; $C'(\xi)$ is the shear modulus; $C_{44}(\xi)$ is the elasticity constant; $\zeta(\xi)$ is the Kleinman constant; $\omega_1, \ldots, \omega_6$ are the weight coefficients. All these values were calculated from the formulas set forth earlier [13,15], while the cohesive energy value was calculated from (Eqs. (1) to 5). The contribution of each square of difference to the objective function value was determined with use of the weight coefficients. The cohesive energy values obtained by the first-principle calculations were used as the reference ones. The point of potential parametric identification is to look for such a set of parameters that provides the calculated values of physical quantities close to the reference ones, which is expressed by the minimum value of the objective function (6). Therefore, solving of the objective function minimization problem will ensure finding of the optimum set of potential parameters for silicon structure description.

To search for the objective function (6) minimum, we used of two algorithms: the Hooke-Jeeves method [16] and the granular radial search method [17]. To ensure the globality of search for both methods, the initial approximation was selected at random within the limits of the acceptable parallelepiped.