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Theoretical investigation of the stability of defect complexes in silicon

Karine Abgaryan* **and Ilya Mutigullin**

Dorodnicyn Computer Center of RAS, Vavilov st. 40, 119333 Moscow, Russia

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* Corresponding author: e-mail kristal83@mail.ru

In this work theoretical investigation of the stability of various defect complexes including vacancies, self-interstitials and their clusters was performed by means of *ab initio* as well as molecular dynamic calculations. Meta-stable defect configurations similar to those observed earlier experimentally were found. Also the software for the molecular dynamic calculations and for the visualization of calculation results was developed. The results of the first-principles calculations were used for the parametrical fitting of Tersoff potential of silicon. Obtained potential was used to perform molecular dynamic calculations of the various configurations of defects in silicon. This approach allowed us to study the dynamics of the atomic system over time and temperature range.

1 Introduction

Defects of the crystal structure of semiconductors are the cause of the substantial change of their properties. Hence the study of silicon defect structure is very important to the production of silicon-based semiconductor elements. One of the ways to produce silicon with photoluminescent properties is irradiation which leads to the creation of various defects in its crystal structure such as point defects, extended defects and their clusters and complexes [1-6]. The mechanics of point defect conglomerates transformation and growth into extended {113} defects is one of the unresolved problems during the ion irradiation of heavy elements into crystal Si. To this moment there are no detailed experimental data about possible cluster types of the point defects in Si, nor detailed theoretical investigations of their stability. In the papers of Fedina et al. [7, 8] the results of experimental investigation via transmission electron microscopy (TEM) of complex self-organizing defect structures in Si crystal during ion implantation by Er atoms with energy of 2 MeV and 600 °C temperature are described. TEM results and calculations with HyperChem computational software have shown that these defect structures are essentially the combination of a splitted dimer and one divacancy arranged in a line in {113} surface. Despite the experimental evidence of such a structure the problem of its stability is not clear and needs additional theoretical clarification.

In this paper we present the results of theoretical investigation of atomic and electronic structure of Si with defects [9] performed in the framework of density functional theory (DFT) [10]. To study the dynamics of point defects and their complexes multiscale modeling methods were applied. For this purpose mathematical model was developed [11] based on molecular dynamics and allowing to define coordinates and velocities of all particles (atoms) of the system. To describe the interatomic interaction the Tersoff potential was used with parameters obtained during the fitting procedure for Si structure. During this procedure results of *ab initio* calculations were used. The developed computational system allows one to perform MD-calculations of Si crystal with point defects and defect clusters and also to make an animated image of the defects' dynamics.

2 Ab initio investigation of point defect clusters

Ab initio calculations were performed with the use of VASP software [12]. For the modeling of the Si crystal without defects periodical cell consisting of 64 atoms was used. The size of the supercell is eight unit cells (2×2×2 = 64 atoms). The Brillouin zone (BZ) sampling was done using the (2x2x2) *k*-point mesh of Monkhorst and Pack and the cutoff energy was chosen to be 250 eV. A relaxation run was terminated when the Hellmann–Feynman forces

on all atoms fell below 0.01 eV/Å, or the total energy variation within one electronic relaxation step fell below 10^{-4} eV. *Ab initio* calculations were performed on the supercomputer of Moscow State University.

This supercell was also used to perform calculations of simple point defects such as vacancy, interstitials, divacancy, Frenkel pair and depleted interstitial atom (DIA). The vacancy was formed by deleting one of the atoms. DIA ($I_{<110>}$) was modelled by placing two Si atoms in one lattice site in the form of dumb-bell with the axis along the <110> direction. The obtained results of the formation energies for studies defects are in a good agreement with previously published data.

On the next step the defect complex consisting of divacancy and DIA was modelled. The structure is shown in Fig. 1: before (a) and after (b) full relaxation.

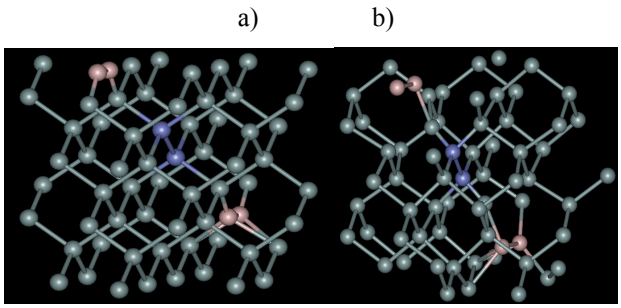

Figure 1 The structure of Si-cell with I-2V defect complex before (a) and after (b) relaxation of atoms.

Formation energies of defects and their complexes were calculated as the difference between the full energy of the system with defect and the energy of ideal Si crystal consisting of the same number of Si atoms as the system with defect. The following formula was used for this purpose:

$$E_f = E_{defect} + \frac{N + \{-n; 1; 0\}}{N} E^N_{cryst} \quad (1)$$

where E_{defect} being the full energy of supercell with defect consisting of N Si atoms minus $-n$ atoms for n-vacancy cluster, +1 atom for $I_{<110>}$, +0 atoms for I-V pair. E^N_{cryst} is the full energy of supercell of ideal Si crystal without defects.

The calculated formation energy of divacancy in the presence of DIA was found to be 4.96 eV. The goal of these calculations was to study the stability of the complex defect consisting of divacancy and two DIA. Therefore, on the next step we studied the most energetically favorable position of DIA in the presence of divacancy (Fig. 2).

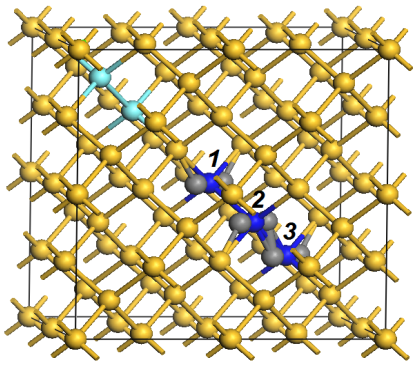

Figure 2 Supercell (2x2x2) containig divacancy and DIA. Two interstitials are in gray, vacancy in the position of depleted atom is in blue, divacancy is in light blue. Positions 2 (3) correspond to various DIA distances from divacancy.

According to our calculations position 1 is the most energetically favorable. It is important to mention that position 1 is a part of defect structure described in the study of Fedina et al. [5, 6]. Therefore the assumption of the fact that the structure consisting of DIA and divacancy is metastable is in agreement with the findings of Fedina.

The problem of the stability of experimentally observed structure needs additional *ab initio* calculations. It is planned to perform calculations of the following systems: two DIAs with a vacancy, two complexes consisting of two DIAs and a vacancy.

3 Molecular dynamics modeling of point defects

To describe interatomic interactions the potential in the form proposed by Tersoff [13] was chosen. For Si this potential includes 12 parameters which one need to define via fitting procedure. For this purpose the goal function containing all potential parameters was minimized. As the result of the fitting the set of parameters was obtained. This set allows to perform semi-empirical calculations of Si structures with the results close to the results of *ab initio* calculations. The Granular Radial Search method [14] was used to find the minimum of goal function [15].

As a result of the Granular Radial Search 200 sets of parameters were found, all providing the value of the goal function equal or less than 0.00001. It is important to mention that structural properties of the material during this procedure are calculated with fixed relative atomic positions. This cannot guarantee that these atomic positions will correspond to the energy minimum for the obtained potential [16]. Hence the relaxation of the structures was performed by means of molecular dynamics [16-18]. It allowed to define atomic positions for the structure under consideration.

This procedure was performed for ideal Si crystal and for Si structure with point defects. The results were in a good agreement with the results of our *ab initio* calculations. To continue our study we are planning to use ob-

tained parameter set to perform molecular dynamics study of extended defect complexes described by Fedina et al.

4 Summary

The results of theoretical investigation of point defects and their clusters are presented. Ab initio calculations in the framework of DFT allowed us to confirm possible stability of the defect structures in Si experimentally observed by Fedina et al. Since these structures are extended and are larger than several lattice cells molecular dynamics method is chosen for their description. For this purpose the Tersoff potential was obtained and prelimenary results of molecular dynamics calculations are in a good agreement with first principles calculations.

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