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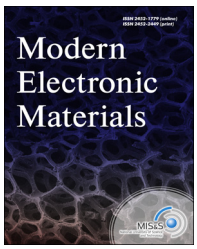

Influence of the *ab-initio* calculation parameters on prediction of energy of point defects in silicon

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Abstract
Point defects play a key role in many microelectronics technologies. Knowledge of the properties of point defects and characteristics of their behavior during ion-beam synthesis of microstructures for use in silicon devices allows one to optimize the conditions of their production, improve their quality and the electronic properties. In this situation, of valuable help in studying the properties of point defects is numerical modeling, especially with the use of quantum mechanical methods based on density functional theory approach. The paper describes a systematic study of the effect of various quantum-mechanical simulation approximations on the calculated energy parameters of defects as applied to simple point defects in silicon. We demonstrate that the choice of the form of the exchange-correlation functional has the strongest effect on the predicted defect formation energy, whereas the variation of the other considered approximations is of secondary importance for simulation predictions.

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Introduction

Study of intrinsic point defects in silicon, their parameters and specific features has been an important field of theoretical and experimental research for many decades. This is due to the key role of point defects in many technologies of microelectronic devices. Knowing the properties of point defects and their

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behavior during the radiation synthesis of microstructures allows optimizing the synthesis conditions of silicon based devices, increasing their quality and improving their electronic properties [1].

Even for simplest point defects in silicon such as vacancies and interstitial atoms a number of their properties and behavior features have not been studied sufficiently. This is largely caused by the complexity of the measurement of point defect parameters even when this is technically possible. Furthermore, some factors specific for semiconductors make additional barriers to the study of point defects. For example, defect parameters in intrinsic silicon may differ from those in *n*- or *p*-type silicon.

In these circumstances, numerical simulation is a powerful tool for the study of point defects, especially simulation using quantum mechanical (*ab-initio*) methods on the basis of the density functional theory (DFT) approach [2]. This method allows assessing point defect formation energies and point defect influence on the electronic properties of the material. The *ab-initio* energy advantage assessments for various point defect configurations and migration barriers provide data on the reliability of semiempirical potential predictions used for the simulation of defect dynamics using classical molecular dynamics methods.

Unfortunately, even the *ab-initio* simulation methods use a number of approximations and simplifying assumptions. The electron density functional theory is only an approximated solution of the multiparticle Schrödinger equation. Further error is introduced by the use of approximate expressions for one of the main parameters treated in this theory, *i.e.* the so-called exchange correlation functional. The most widely used approximations are currently as follows: local electron density (LDA) [2] and generalized gradient (GGA) [3] appriximations. Another ambiguity is caused by the method of describing the interaction between the valence electrons and the strongly bonded electrons in the material. It also uses two main approaches, *i.e.* the projector augmented wave (PAW) method [4] or the use of pseudo-potentials of which the most widely used are the so-called ultrasoft (US) pseudo-potentials [5]. Along with the abovementioned approximations, calculation accuracy also depends on the used simulation cell size, the choice of parameters for numerical equation solution, etc. However, the latter errors can be (and must be) minimized by adequately choosing calculation parameters (see *e.g.* [6,7]), whereas the errors related to the choice of the exchange correlation functional or the description of valence electron interaction with inner shells of ions are fundamentally unavoidable.

According to the practice of applying various approximations used in the density functional theory, calculated point defect energies often prove to depend on the choice of simulation parameters. To assess the overall accuracy of the DFT method for each specific case one should compare calculated point defect parameters obtained using various approximations. Unfortunately, because of the high complexity of *ab-initio* calculation methods there are only few, if any, systematic studies of the effect of approximation type on the predicted point defect parameters.

The aim of this work is to study the effect of various approximations used for *ab-initio* quantum mechanical simulations on point defect energy predictions for several simplest point defects in silicon. The variable parameter was primarily the type of the exchange correlation approximation used. For some calculations we also varied the method of describing valence electron interaction with inner shells of ions and the calculation cell sizes. To demonstrate the practical applicability of the simulation data we compared the results for an interstitial atom in silicon for *ab-initio* calculations and for semiempirical potentials.

Simulation method

The electron density functional theory calculations were carried out using the Vienna *ab-initio* Simulation Package (VASP) and the GGA and LDA approximations for exchange correlation potential. The interaction between the valence electrons and the strongly bonded electrons of ion core was described using US pseudo-potentials and the PAW method. The cutoff energy in the wave function decomposition into plane waves was selected to be at least 300 eV. For the calculations we used the *k*-grid of Monkhrost-Pack type. The grid density depended on the calculation cell size and varied from $8\times8\times8$ points for 8-atom cells to $2\times2\times2$ points for the cells with 216 or more atoms. These selected calculation parameters are sufficient for the convergence of the calculation results. The numerical relaxation of atomic configurations with defects was conducted until the maximum force affecting the atom fell below 0.01 eV/nm.

For point defect simulation, we used cubic periodical cells containing 8, 64 or 216 silicon atoms. Interstitial atoms were simulated using up to 576 atom cells. The initial configurations of vacancies and divacancies in the silicon crystalline lattice were constructed by removing the required number of atoms from cell sites and the initial configurations of interstitial atoms were constructed by placing an additional silicon atom to obtain a configuration that is close to the required one.

To assess the effect of 8 or 64 atom calculation cell size on elastic relaxation we allowed adjustment of the cell size for minimizing the total energy. For large cells the size was constant because their relaxation due to the addition of point defects is negligible.

The formation energy E_D^f of an arbitrary type point defect ($D=V$ for vacancies, 2 V for divacancies and I for interstitial atoms) was calculated using the following formula:

$$E_D^f = E_D^{\mathrm{tot}} - E_0^{\mathrm{tot}} + (n_V - n_I)E_c,$$

where E_D^{tot} and E_0^{tot} are the total lattice energies for defect containing and defect free lattices, respectively, $E_c=E_0^{\mathrm{tot}}/N$ is the energy per one atom in the perfect lattice, N is the number of lattice sites in calculation cell and n_V and n_1 are the numbers of empty sites and interstitial atoms, respectively, in defect containing lattices.

The binding energy of two vacancies in a divacancy was calculated using the formula

$$E_{2V}^b = 2E_V^f - E_{2V}^f,$$

or (for adjusted size cells) as the difference of the total vacancy-containing cell energies at the maximum possible