Computing Diffusion Coefficients of Intrinsic Point Defects by Atomistic Simulations

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We present a new method to identify and track intrinsic point defects in a silicon crystal in a molecular dynamics simulation. If the canonical ensemble is employed, the resulting trajectory can be used to compute the diffusion coefficients of defects for a prescribed temperature. A fit of these values for different temperatures to an Arrhenius–type function gives the temperature dependence of the diffusion coefficient over the whole range of interest. For this purpose, we performed simulations employing the Stillinger–Weber potential as well as the Tersoff potential. We were able to improve the accuracy of the approximation of the diffusion coefficients for self-interstitials and vacancies computed by Sinno [2] and Tang et al. [5].

Keywords: Point defects, Interstitials, Vacancies, Diffusion Coefficient, Molecular Dynamics, Stillinger–Weber, Tersoff

I. INTRODUCTION

Industrial fabrication of semiconductor devices requires a high quality of the base material. Hence, the growth process of crystalline silicon has to be improved continuously. During the growth process, the formation of the crystal is influenced by the appearance of point defects in the lattice. These point defects can develop into microdefects during the annealing process which affect the quality of the crystal. Thus, the aim is to avoid the formation of such defects already during the crystal growth process. This can be achieved by optimizing the temperature distribution in the furnace and the pull velocity of the growing crystal. Both parameters affect the defect distribution. However, their optimal control is a very difficult task. To this end, simulations of the whole crystal growth process for various parameter sets are necessary. This is subject to current research. Such simulations compute the defect distribution in the growing crystal as a measure of the crystal quality. First attempts in this direction were made by Brown et al. [1, 2]. Here, stationary results for the defect distribution were computed. Recent simulations [3, 4] are also able to investigate the evolution of the defect distribution during the growth process.

Such macroscopic simulations of the growth process highly depend on the parameters which describe the material properties of silicon. Here, the most important parameters are the diffusion and the concentration coefficients of the point defects. However, due to the high temperatures in the furnace, it is very difficult to measure them experimentally. Reliable experimental data only exist for the *product* of diffusivity and concentration. Hence, one might resort to atomistic simulations in order to determine the temperature dependence of the specific material properties. To this end, long time intervals and large system sizes are required for a microscopic molecular dynamics simulation. These are necessary to ensure statistical convergence of any macroscopic parameter to be derived. The computational costs for such simulations still are very high, even with up-to-date parallel computers. Here, since the use of ab initio methods is not affordable yet, simpler but faster approximations to the forces in the crystal are applied. First attempts using the tight-binding molecular dynamics (TBMD) method, where the forces are calculated by directly diagonalizing the one-electron Hamiltonian matrix, were made with promising results [5]. But this method still is restricted to short time intervals. Molecular dynamics simulations with semi-empirical potentials are able to provide longer time intervals up to several nanoseconds. Here, analytic potential functions are fitted to reproduce specific properties of the material. It is unclear to what extent such potentials can yield reasonable results for other properties, and corresponding results have to be used with care.

In this paper we describe a new method to identify and track intrinsic point defects in a silicon crystal during a molecular dynamics simulation. Here, we compute the bond order of each atom and test it for a criterion that distinguishes lattice atoms from interstitials and vacancies. We apply the method to determine the temperature dependence of the diffusion coefficients of the point defects. To this end, trajectories of the point defects are calculated for different temperatures. From these trajectories the diffusion coefficients for the respective temperature can be computed. To obtain the temperature dependence continuously over the whole range of interest, an Arrhenius–type function is fitted to the computed data.

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This result can then be used in a macroscopic simulation of the whole growth process with the aim to improve the industrial fabrication of silicon crystals [6].

The remainder of this paper is organized as follows: In Section II, we describe our method to identify and track point defects during the simulation and explain how the diffusion coefficients can be computed from the point defect trajectories. In Section III, we present the results obtained with our method and compare it to the results found in the literature. Finally, we present some conclusions and discuss open questions in Section IV.

II. METHOD

A. Point Defects

Let us consider a silicon crystal on the atomistic scale. There are two types of intrinsic point defects: Self-interstitials and vacancies. Self-interstitials are additional silicon atoms which are not located at a crystal lattice point. Vacancies are defined by a missing lattice atom. The identification of these defects during an atomistic simulation is a challenging task since they cannot be identified by single particles which would be easy to track. Interstitials often exchange their place with a lattice atom, hence any atom can become an interstitial during a simulation and vice versa. Vacancies are not particles in the classical sense, since they are defined by the absence of a lattice atom. This characterization makes a check of the whole lattice inevitable; i.e., the only possibility to detect these defects is by testing all atoms in the simulation domain for errors of the lattice structure. To this end, one needs a description of the lattice on the atomistic level.

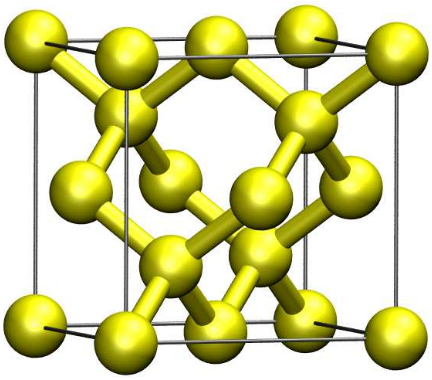

FIG. 1: Unit cell of the diamond structure of silicon.

Silicon crystallizes in the so-called diamond structure; i.e., the four nearest neighbors of each atom form the vertices of a tetrahedron, see Fig. 1. As can be seen in Fig. 2, the radial distribution function of this type of lattice structure has a distinct peak around the distance of adjacent atoms. This property can be used for

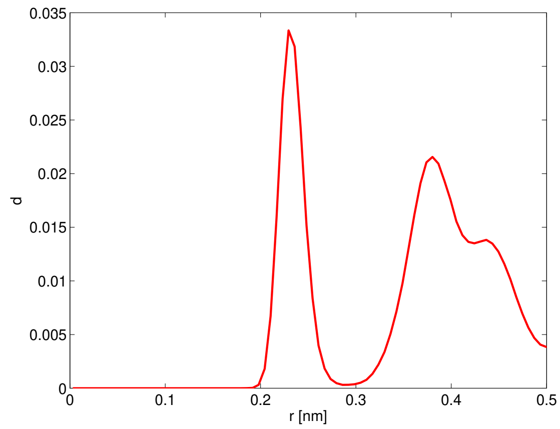

FIG. 2: Radial distribution of particles in a perfect silicon crystal.

a simple but efficient test for errors in the local structure: In the faultless crystal, each atom should have exactly four neighbors within the characteristic distance of $r_{nb} = 0.29\ nm$. The number n of neighbors within this distance is the so-called *bond order*. A deviation of this bond order from the value gives a hint on a defect.

Since we want to identify special intrinsic point defects we need to specify which deviations will be caused by the different defects. To this end, the following holds: A self-interstitial is an additional silicon atom which does not belong to the lattice. Hence, the bond order of all lattice atoms which are direct neighbors of this interstitial is increased by one. The interstitial itself then typically has six or more neighbors within the sphere of radius r_{nb}. It therefore can efficiently be identified by this property. Vacancies cause deformations of the local structure, since the neighboring atoms tend to move towards the empty space. Thus, they can be localized by looking at the bond orders of neighboring atoms. If at least two neighboring atoms with a significant deviation (larger than one) of their bond order are found, then there is a vacancy present. Its position is approximated by averaging the locations of the respective neighboring atoms. In summary, all atoms (lattice, interstitials) can be classified by their bond order n:

$$\begin{aligned} n = 4 &\quad : \text{ lattice atom} \\ n > 5 &\quad : \text{ interstitial} \\ \text{at least 2 neighbors with } n > 5 &\quad : \text{ vacancy} \end{aligned} \tag{1}$$

This criterion makes an identification of point defects possible for each single time step. The aim, however, is to track a defect during the whole simulation. To this end, it is helpful that the defect concentrations in crystalline silicon are very low at the temperatures of interest. Thus, simulations with more than one point defect are not necessary. It is sufficient to identify a single point defect and localize it at each time step. This directly leads to a trajectory of the defect. In principle, more than one defect of the same type can be treated in one simulation as well. Problems only occur when two defects cross each others trajectory. Then, the defects might mutually be assigned to the wrong trajectory. But due to the stochastic nature of the defect movement and the indistinguishability of defects of the same type, this has no effect on the computation of macroscopic values.

How can the above described procedure for detecting and tracking intrinsic point defects during an atomistic simulation be efficiently implemented? First, one has to determine the bond order of each atom in the simulation domain at each time step. For this purpose, all neighbors of an atom within a sphere of radius r_{nb} have to be found and counted. The naive approach of checking the distance between all possible pairs of atoms would be of order $\mathcal{O}(N^2)$, if N denotes the total number of atoms. However, one can use the well-known linked-cell technique [7, 8] in order to reduce the complexity to $\mathcal{O}(N)$. To this end, one divides the domain into cubic cells of side length $L \geq r_{nb}$ and assigns all particles to their associated cells. In order to find all neighbors of an atom within the prescribed distance r_{nb} it is then sufficient to consider only the particles which lie in the same or adjacent cells. After the bond order is determined for all particles, the point defect criterion (2) is used to identify interstitials and vacancies for the current time step. Due to thermal fluctuations in the crystal, sometimes also lattice atoms are wrongly classified as interstitials or vacancies. But these cases are rare and of stochastic nature. They are easily eliminated by verifying whether the detected position can belong to the traced trajectory or not. To this end, simply the distance to the position of the defect at the last time step is checked.

A simulation of a silicon crystal with a point defect then leads to the trajectory of this defect. Fig. 3 shows an example of such a trajectory over a period of 2.5 ns. Since the molecular dynamics simulation uses periodic boundary conditions, a point defect can leave the domain at one side and reenters it at the opposite side. In order to use such a trajectory for the computation of macroscopic diffusion coefficients it first has to be corrected with respect to this boundary conditions as follows: If the point defect leaves the domain at one side and reenters it at the opposite side this has to be accounted for by adding/subtracting one side length of the domain to/from the respective coordinate. The resulting trajectory is then smoothed by a low-pass filter in order to reduce the effects of the small spatial fluctuations of the point defect, see Fig. 3. This continuous and smooth trajectory can then be used to compute the diffusion coefficient of the point defect by means of statistical mechanics.

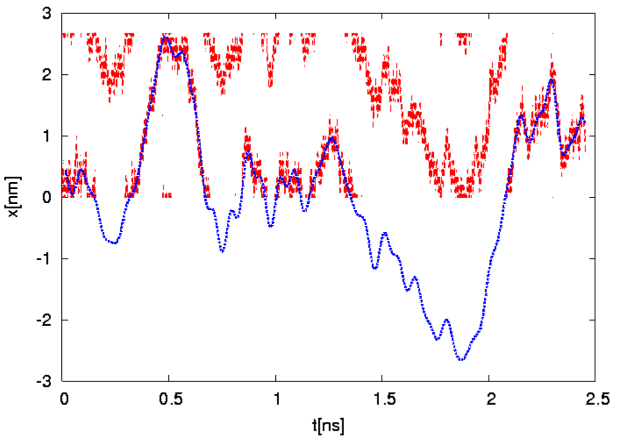

FIG. 3: X-coordinate of computed trajectory and periodically corrected and smoothed trajectory of a vacancy.

B. Diffusion Coefficient

The aim is now the computation of temperature-dependent macroscopic material properties like the diffusion coefficients of self-interstitials and vacancies. Since we perform atomistic simulations, we have to use methods from statistical mechanics in order to compute macroscopic parameters from microscopic values. All simulations are performed in the canonical ensemble, i.e. at constant temperature. Here, macroscopic values can be obtained by averaging the microscopic values with the Boltzmann factor, i.e.

$$\langle A \rangle := \frac{\int A(\mathbf{x},\mathbf{p}) e^{-\beta H(\mathbf{x},\mathbf{p})} d\mathbf{x}\ d\mathbf{p}}{\int e^{-\beta H(\mathbf{x},\mathbf{p})} d\mathbf{x}\ d\mathbf{p}} \text{ with } \beta := \frac{1}{k_B T}, \quad (2)$$

where A is the microscopic value, H denotes the microscopic energy of the system, $\mathbf{x}$ and $\mathbf{p}$ are the positions and momenta of the particles, T is the temperature and k_B denotes the Boltzmann constant. In this sense, the diffusion coefficient is directly related to the spatial motion of the particles or point defects. Einstein first derived that the diffusion coefficient $D_{I,V}$ (I for interstitial, V for vacancy) can be written as

$$D_{I,V} = \frac{1}{6} \frac{\partial}{\partial t} \langle |\mathbf{x}_{I,V}(t) - \mathbf{x}_{I,V}(t_0)|^2 \rangle \quad (3)$$

where $\mathbf{x}_{I,V}(t)$ is the position of a interstitial or vacancy at time t. From this equation it follows that

$$\langle |\mathbf{x}_{I,V}(t) - \mathbf{x}_{I,V}(t_0)|^2 \rangle \propto t, \quad (4)$$

since $D_{I,V}$ is a constant. Hence, we can write

$$\langle |\mathbf{x}_{I,V}(t) - \mathbf{x}_{I,V}(t_0)|^2 \rangle = c_0 + d \cdot t \quad (5)$$

with constants c_0 and d. The diffusion coefficient can then be calculated as $D = d/6$.

Since the computation of the associated high dimensional integral in (5) is not possible in appropriate run time, one has to resort to an approximation. This can be done as follows: A molecular dynamics simulation results in a discrete trajectory of the respective point defect, i.e. a discrete set of locations $\mathbf{x}^m_{I,V}(t_0), \mathbf{x}^m_{I,V}(t_1), \ldots, \mathbf{x}^m_{I,V}(t_n)$ at times $t_i, i = 1, \ldots n$. From these locations the discrete function

$$r^m_{I,V}(t_i) := \left|\mathbf{x}^m_{I,V}(t_i) - \mathbf{x}^m_{I,V}(t_0)\right|^2$$

can be calculated. This function deviates from the expected values

$$\langle|\mathbf{x}_{I,V}(t_i) - \mathbf{x}_{I,V}(t_0)|^2\rangle = c_0 + d \cdot t_i$$

by a stochastic error. Using the Ergoden hypothesis, equation (3) is equivalent to

$$D_{I,V} = \lim_{t\to\infty} \frac{1}{6(t-t_0)} |\mathbf{x}_{I,V}(t) - \mathbf{x}_{I,V}(t_0)|^2. \qquad (6)$$

Of course, this expression cannot be computed either. But for the discrete function $r^m_{I,V}$

$$\lim_{n\to\infty} \frac{r^m_{I,V}(t_n)}{t_n - t_0} = d.$$

holds. If we now fix t to a large value and thus neglect the limes we obtain an approximation of the diffusion coefficient. Due to the stochastic nature of the point defect movement, the error of this approximation is quite large for computationally achievable values of t. Instead, we use the computed time-discrete function $r^m_{I,V}(t_i), i = 1, \ldots n$, to approximate the line $c_0 + d \cdot t$ by a least square fit. Then the stochastic errors are eliminated if the computed trajectory is long enough. The result is an approximated slope $\tilde{d}$ and an approximative diffusion coefficient $\tilde{D} = \tilde{d}/6$. In practice, time intervals of several nanoseconds have shown to give acceptable results. However, more accurate predictions — supposing that the potential correctly describes the investigated property — will require simulation times of some picoseconds in the case of point defect diffusion.

Now, each of the molecular dynamics runs leads to a trajectory of a point defect and to a value for the diffusion coefficient at a prescribed temperature. In order to use the computed diffusion coefficients in macroscopic process simulations their values are needed at arbitrary temperatures. To this end, we have to provide an analytical function which then is fitted to the computed values at the respective temperatures.

We proceed as follows: Experimental methods only allow the measurement of the product of the equilibrium defect concentration $C_{I,V}$ and the diffusivities $D_{I,V}$ [9]. Gösele et al. [9] specify these quantities as

$$C_I D_I = 914 \exp\left(-\frac{4.84\ eV}{k_B T}\right) cm^2/s$$

$$C_V D_V = 0.6 \exp\left(-\frac{4.03\ eV}{k_B T}\right) cm^2/s.$$

These formulae are rather reliable in the case of interstitials whereas they are still controversial in the vacancy case. The individual values for the concentrations and diffusivities are not known. But these experimental results together with further theoretical assumptions suggest an Arrhenius behavior of the point defect diffusion coefficients, i.e.

$$D_{I,V} = D^0_{I,V} \exp\left(-\frac{E^m_{I,V}}{k_B T}\right), \qquad (7)$$

see also [5, 10, 11]. Here, $D^0_{I,V}$ denotes the diffusivity prefactor and $E^m_{I,V}$ the migration energy. These parameters can be determined by a least square method to fit function (7) to the computed data points of the diffusion coefficients.

III. RESULTS

A. Details of the molecular dynamics simulations

In order to determine the temperature dependence of the diffusion coefficient of intrinsic point defects in a solid material, molecular dynamics runs at constant temperature in a domain with periodic boundary conditions are necessary. Since the temperature dependence of the density can be neglected for most solids, the (NVT)-ensemble can be employed. To this end, we used the Nosé thermostat [12] for the coupling to a heat bath. There exist two potentials for the condensed phases of silicon: One by Stillinger and Weber [13] and one by Tersoff [14–17]. A simple pair potential like the Lennard-Jones interaction, which is typically used for liquefied noble gases, is not sufficient for the simulation of covalent systems. Hence, both, the Stillinger–Weber potential and the Tersoff potential, consist of two- and three-body terms. The general form is

$$U(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = \sum_{\substack{i,j \\ i>j}}^{N} f_2(\mathbf{x}_i, \mathbf{x}_j) + \sum_{\substack{i,j,k \\ i>j>k}}^{N} f_3(\mathbf{x}_i, \mathbf{x}_j, \mathbf{x}_k)$$

where f_2 is a two-body function, f_3 a three-body function and N the total number of atoms in the simulation domain. The two potential forms differ, however, in their exact definition of f_2 and f_3. Furthermore, these functions are fitted to different properties of silicon. In the case of the Stillinger–Weber potential the incorporated parameters were chosen to stabilize the diamond structure at low pressure and to give good agreement with experimental data for the melting point and the liquid structure. The parameters of the Tersoff potential are fitted to correctly reproduce cohesive energies, the bulk modulus and the bond length in the diamond structure. In [16] the parameter set was improved to give better results for the elastic properties of silicon. However, the Tersoff potential does not reproduce the correct melting point [16]. Therefore, its use to determine temperature dependent properties is controversial. We used both

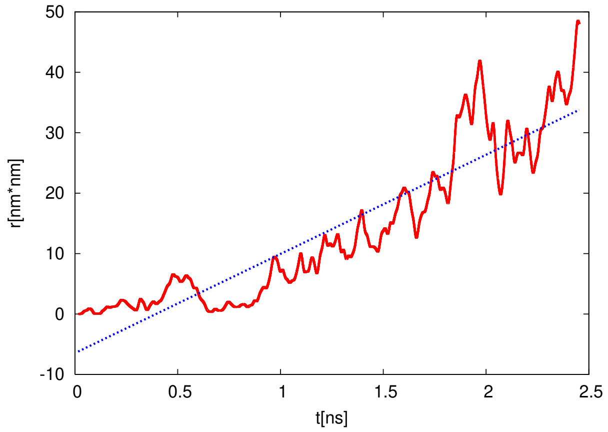

FIG. 4: Function $r_{I,V}^m(t_i)$ of a trajectory of a vacancy and fitted line.

potentials for both types of intrinsic point defects. A comparison of the obtained results will be given in the following subsections.

Both potentials are short-ranged. Hence, one can use the linked-cell method for the efficient evaluation of the forces. For the three-body terms one has to find all triples of particles where at least two of the three possible distances between the three particles are smaller than the potential-specific cut off. This triple search can be implemented by an additional cycle through the neighboring cells of the linked-cell structure for all pairs of particles.

Most of the computations concerning point defects in the literature so far were performed using a periodic supercell which contains 216 or less atoms [5, 10, 11]. Furthermore, the simulation times ranged from ps to ns [5, 11]. We were able to increase the system size to 1000 particles in a periodic box of 2.67 nm and reached simulation times up to 27 ns. Our initial configuration was always a perfect tetrahedral crystal with a density of 2.44 g/cm^3. The considered point defect was introduced at the beginning of the simulation by either adding a silicon atom randomly or by removing one of the lattice atoms. All simulations were done in the (NVT)-ensemble. The diffusion coefficients were computed for interstitials and vacancies with both, the Stillinger–Weber and the Tersoff potential.

B. Diffusion coefficients

Each molecular dynamics simulation at a prescribed temperature results in a trajectory of the considered point defect. Fig. 3 showed an example of a trajectory of a vacancy for a small time period. Then, from each trajectory the function $r_{I,V}^m(t_i)$ is computed, see Fig. 4. Finally, a least square fit of this function gives a line whose slope is directly proportional to the diffusion coefficient at the prescribed temperature. Table I shows the results of this approach for both types of defects and both types of potentials. These data points then were

TABLE I: Computed diffusion coefficients.

$T\ [K]$	$D_I^{SW}\ [\frac{cm^2}{s}]$	$D_I^{TER}\ [\frac{cm^2}{s}]$	$D_V^{SW}\ [\frac{cm^2}{s}]$	$D_V^{TER}\ [\frac{cm^2}{s}]$
1258.9	$1.535 \cdot 10^{-5}$	–	$0.461 \cdot 10^{-5}$	$0.043 \cdot 10^{-5}$
1384.8	$1.166 \cdot 10^{-5}$	$0.029 \cdot 10^{-5}$	$0.294 \cdot 10^{-5}$	$0.108 \cdot 10^{-5}$
1435.1	–	$0.190 \cdot 10^{-5}$	–	–
1510.7	$3.100 \cdot 10^{-5}$	$0.046 \cdot 10^{-5}$	$0.587 \cdot 10^{-5}$	$0.273 \cdot 10^{-5}$
1586.2	–	$0.313 \cdot 10^{-5}$	–	–
1636.6	$7.144 \cdot 10^{-5}$	$0.610 \cdot 10^{-5}$	$1.054 \cdot 10^{-5}$	$1.194 \cdot 10^{-5}$
1762.4	$8.678 \cdot 10^{-5}$	$1.038 \cdot 10^{-5}$	$0.346 \cdot 10^{-5}$	$1.745 \cdot 10^{-5}$
1888.3	–	–	–	$1.266 \cdot 10^{-5}$

TABLE II: Computed diffusivity prefactors and migration energies.

Defect type	Potential	$D^0\ [cm^2/s]$	$E^m\ [eV]$
Interstitial	Stillinger–Weber	$1.45 \cdot 10^{-2}$	0.78
Interstitial	Tersoff	2.13	1.85
Vacancy	Stillinger–Weber	$1.26 \cdot 10^{-4}$	0.12
Vacancy	Tersoff	0.55	1.27

used to fit the parameters of the Arrhenius–type function (7) to give the temperature dependence over the whole range of interest. Fig. 5 and Fig. 7 show the data points and the fitted line in a semi-logarithmic graph for self-interstitials and vacancies, respectively. The resulting values for the diffusivity prefactors and migration energies are given in Table II. A comparison with the values found in the literature [5, 10, 11] shows good agreement, see Fig. 6 and Fig. 8. The Stillinger–Weber potential predicts a defect migration which is dominated by self-interstitials for higher temperatures ($> 1600\ K$), whereas for lower temperatures the vacancy migration is larger. We were able to improve the accuracy of the results obtained by Sinno [2] with the Stillinger–Weber potential by an increase of the system size of the molecular dynamics simulations and a larger number of simulations at different temperatures. Compared to the results given in [2], we obtained an overall higher migration for self-interstitials and similar results for the migration energy and diffusivity prefactor. In the vacancy case, the migration energy differs more significantly from [2]. Here, our results are similar to those from Tang et al. [5]. The Tersoff potential, however, yields larger values for both the migration energy and the diffusivity prefactor. This is surprising since the Tersoff potential has a melting point which is about twice as high as the experimental value. Hence, the temperatures of our simulations, which are near the experimental melting point of silicon, lie far away from the melting temperature of the Tersoff potential. Here, however, point defect migration should be small. One can conclude that, although both potentials result in comparable results, the use of the Tersoff potential for measuring temperature-dependent properties is at least questionable.

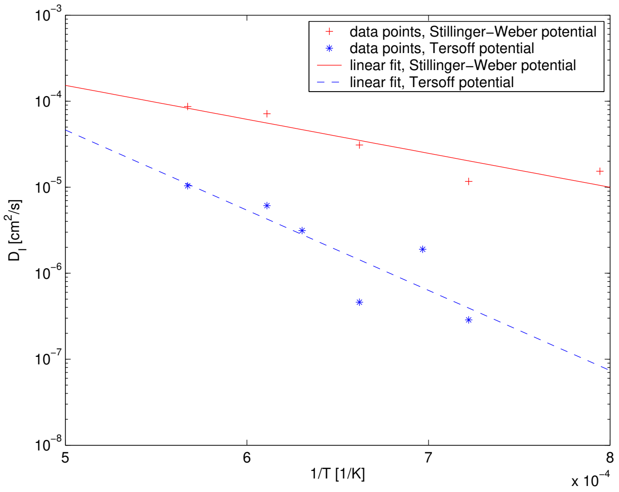

FIG. 5: Temperature dependence of the diffusion coefficient for self-interstitials.

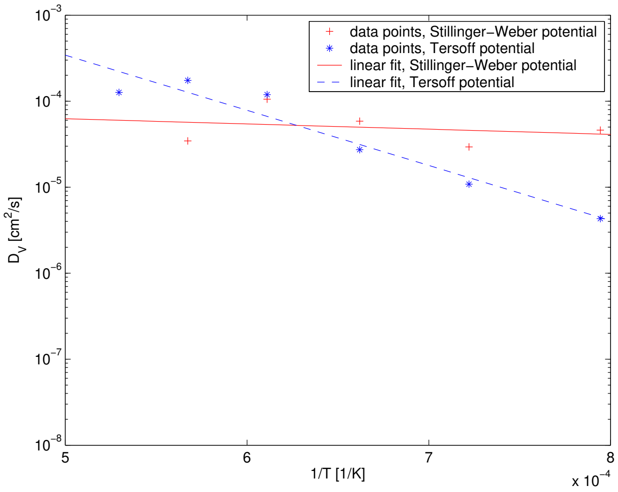

FIG. 7: Temperature dependence of the diffusion coefficient for vacancies.

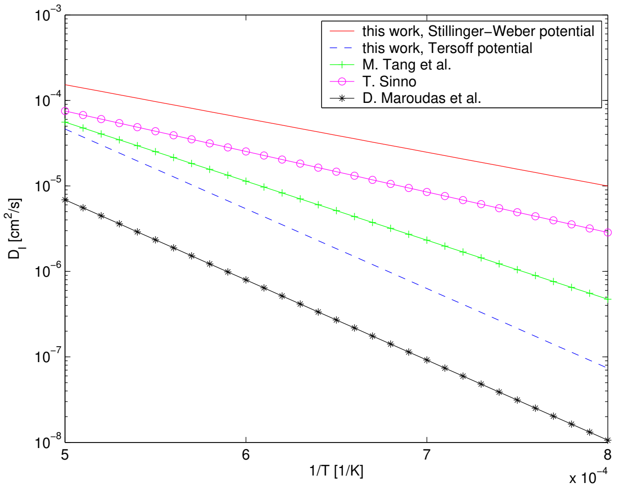

FIG. 6: Comparison of our results with the ones found in the literature for self-interstitials.

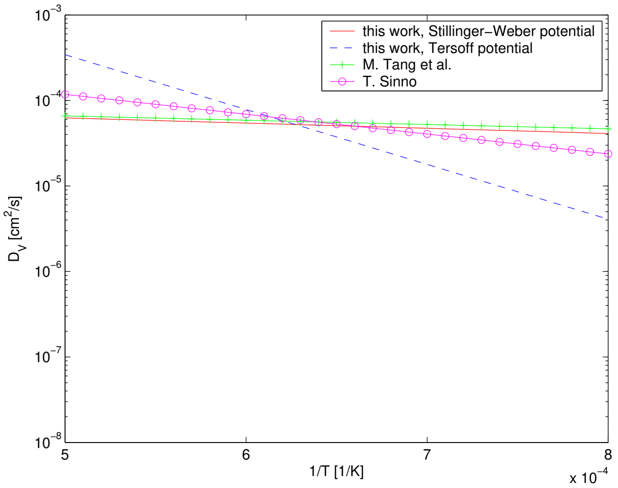

FIG. 8: Comparison of our results with the ones found in the literature for vacancies.

The major problem of the determination of macroscopic quantities by atomistic simulations is the huge computational effort which is necessary to get statistical reasonable results. Due to the stochastic nature of the point defect movement, long simulation times are inevitable in order to reduce the error sufficiently. This effect can clearly be seen in Fig. 4, where the measured function $r^m_{I,V}(t_i)$ shows large fluctuations around the mean square displacement $\langle(\mathbf{x}_V(t_0) - \mathbf{x}_V(t))^2\rangle$. Such long simulation times, however, cannot yet be reached. Therefore, the existing methods today only allow for a rough computation of the temperature dependence of the diffusion coefficient and cannot yield more exact predictions so far.

IV. CONCLUSIONS

To improve the quality of semiconductor base material, macroscopic simulations of the whole silicon crystal growth process are necessary. For these simulations, information on the properties of silicon are needed which cannot be gained from experimental measurements. Therefore, we have to resort to atomistic simulations to compute these properties.

In this paper we computed the temperature dependence of the diffusion coefficients of intrinsic point defects in a silicon crystal. We presented a new method to identify the defects during the simulation. To this end, we test the bond orders of all atoms in the simulation domain for specific criterions. This enables us to track the point defects during the simulation in a completely automatic way. From the resulting point defect trajectories we then compute the diffusion coefficient at a specific temperature. Finally, an Arrhenius–type function is fitted to the diffusion coefficients obtained for different temperatures.

The major problem of this procedure is the long time interval of the simulation necessary to get reliable results from the statistical data and, thus, the computational effort involved. So far, only simulations with semi-empirical potentials are capable to reach sufficiently large time intervals. Ab initio calculations for computing point defect diffusivities are out of question by today. Anyway, our approach allows in principle to derive macroscopic quantities in sufficient quality as long as an appropriate potential function is available and a large and fast computer is used.

V. ACKNOWLEDGMENTS

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