

Effect of the Interatomic Si-Si-potential on Vacancy Production during Ion Implantation of Si.

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Collision cascades in crystalline silicon due to impinging 10 eV - 1 keV Si atoms are simulated using molecular dynamics methods. The simulations are carried out for 30 - 100 events to obtain representative statistics for production of different types of vacancies. The results are used to examine the dependence of vacancy production on the interatomic Si-Si potential between the colliding atoms. The dependence of the number of vacancies was found to be sensitive to the form of the potential well but not to the repulsive potential. The results suggest that within the heavily damaged volume of the collision cascade an interatomic potential with somewhat narrower well than that of the commonly used Stillinger-Weber potential should be used to simulate the vacancy production in silicon.

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1. INTRODUCTION

Processes that produce damage in crystalline silicon during ion implantation have been studied extensively, see e.g. refs. [1-6]. Simulations of vacancy production processes in solids have been carried out using various binary-collision-approximation (BCA) and molecular dynamics (MD) simulation methods [7]. Only rough estimates on the number of vacancies can be obtained with the BCA methods in the framework of the empirical Kinchin-Pease equation [7]. Molecular dynamics simulation methods are required in realistic simulations of collision cascades.

In MD simulations, defect formation has typically been estimated on the basis of a single or a couple of cascade simulations (see e.g. refs. [8,9]). However, this leads to highly unreliable results, as illustrated by fig. 1. In fig. 1 the number of vacancies in ten different collision cascades produced by a 300-eV Si atom recoiling in crystalline silicon (c-Si) are shown as a function of time along with the average value calculated from 100 events (see below).

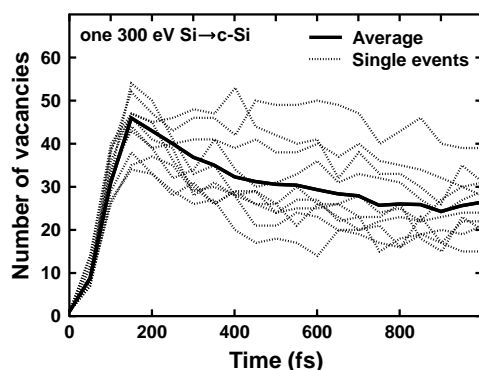


FIG. 1. Number of vacancies produced by 300 eV recoils with randomly selected initial recoil directions. Ten individual events and the average calculated from 100 events are shown.

In previous works where processes in c-Si have been simulated with MD methods employing classical potentials, the number of defects obtained has been found to be significantly higher than experimental values [10]. Low-energy processes in small atom clusters can be more real-

istically simulated using *ab initio* MD methods [11,12] than with classical MD methods. However, *ab initio* MD simulations are still far too slow to handle processes involving interaction energies higher than a few eV or systems with more than a few hundreds of atoms. Therefore, a better understanding of classical MD simulation methods is desirable to obtain more realistic defect concentrations in simulations of collision cascades, which involve keV energies and several thousands of atoms.

This work was undertaken to study how the vacancy production during the implantation of 10 eV - 1 keV Si atoms into c-Si depends on the interatomic Si-Si potential.

2. PRINCIPLES OF THE SIMULATIONS

The MD simulations were carried out using a modified version of the computer code used previously in our laboratory for the simulation of slowing down of low-velocity recoils (energy less than 100 eV/amu) produced in thermal neutron capture reactions [13].

The potential employed in the simulations was the Stillinger-Weber three-body potential commonly used in simulating the structure of c-Si [14]. To obtain a realistic potential at small separations ($r < 1.7$ Å), the Stillinger-Weber potential was splined between $r = 1.7$ and 2.0 with the repulsive potential.

The simulation of a collision cascade was initiated by selecting a recoiling atom among silicon atoms in one corner of the simulation cell, and giving it a recoil velocity in an isotropically chosen direction in one quadrant. A recoil energy of 1 keV was selected to test the effect of the repulsive potential. To test the effect of the potential well separately, lower energies were chosen. However, in order to obtain statistically significant results it is important that more than only a few vacancies are produced for one recoil event. Therefore, a recoil energy of 300 eV which was found to yield between 20 and 50 vacancies in one recoil event was chosen.

The size of the simulation cell was set to be large enough to contain the entire collision cascade. For 1 keV recoils this amounted to a cell of $76 \times 76 \times 76$ Å³ with 21952

atoms and for 300 eV recoils to a cell of $54 \times 54 \times 54$ ³ with 8000 atoms.

The initial velocities of the atoms in the simulation cell were chosen randomly according to the Maxwell velocity distribution. Thermal movement of the atoms in the cell was simulated for 100 fs at 300 K to obtain realistic thermal displacements.

The time step in the simulations was initially 0.1 fs and was made longer during the simulation as the recoil atom slowed down. The longer time steps were selected so that the fastest atom in the simulation cell did not move more than 0.1 during one time step. The algorithm employed to solve the equations of motion was a modified Beeman algorithm presented in ref. [15].

The temperature of the outermost 3 atom layers was scaled down to 300 K at regular intervals to realistically dissipate energy from the simulation cell. To prevent the entire cell from starting to move due to extra momentum obtained from the recoil atom, the sum of the vector momenta of the atoms in the outermost layer was also scaled down to zero. The scalings also prevented kinetic energy from being reflected back from borders of the simulation cell.

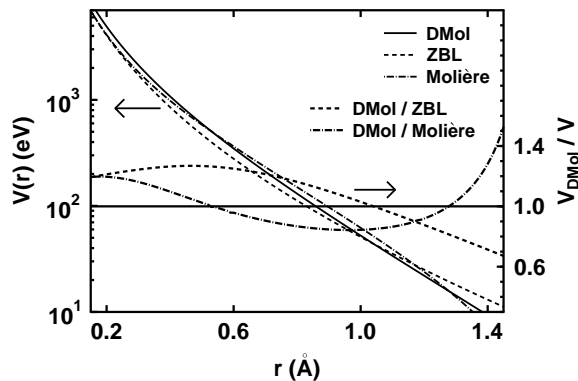


FIG. 2. Interatomic repulsive Si-Si potentials used in the simulations of vacancy production.

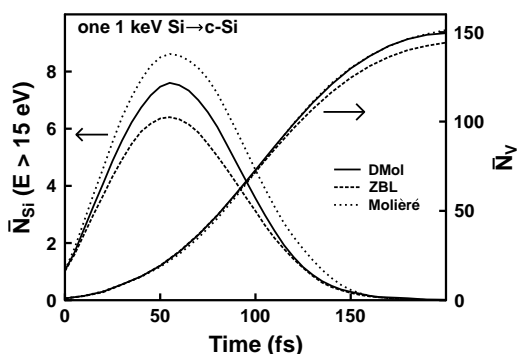


FIG. 3. Average numbers of recoiling Si atoms with energies greater than 15 eV ($\bar{N}_{Si}(E > 15 \text{ eV})$) and number of vacancies (\bar{N}_V) produced in the slowing down process of one 1-keV Si atom in c-Si. The numbers are averages calculated from 50 simulation events for the three potentials shown in fig. 2.

Vacancies were detected in several ways during the simulations. The total number of vacancies was calculated by counting all original lattice sites that were empty. For

each located empty site the nearest-neighbour sites were examined for emptiness, yielding the numbers of mono-, di-, tri- etc. vacancies. A site was defined as empty if it did not contain any atom within a radius of 1.2, corresponding to the half of the nearest-neighbour distance.

The number of atoms with energies greater than a threshold energy of 15 eV (the minimum value of E_d in the Kinchin-Pease equation, see below) was also calculated.

3. RESULTS AND DISCUSSION

The dependence of the number of vacancies on the repulsive potential was examined by simulating 50 1-keV recoil events for three different potentials. The potentials used were the universal ZBL potential [16], a modified Molière potential [17], and a potential obtained from *ab initio* calculations using the commercial DMol program [18,19]. The potentials are shown in fig. 2, and the results in fig. 3.

Although the number of secondary recoils with energies greater than 15 eV (corresponding to the minimum energy required for the formation of a Frenkel pair in c-Si [20,21]) differ significantly for the three potentials the number of vacancies produced does not show any statistically significant dependence on the repulsive potential.

To test the effect of the form of the potential well on vacancy production, the parameters S , p , m_1 and m_2 in the two-body-part of the Stillinger-Weber-potential

$$V_2(x) = \begin{cases} S\epsilon A(Bx^{-p} - m_1)e^{m_2/(x-a)} & 0 < x < a \\ 0, & x > a, \end{cases} \quad (1)$$

were modified. The unmodified values for the parameters are $S = m_1 = m_2 = 1$ and $p = 4$.

The modified values were selected so that the middle point of the well is at the equilibrium separation of 2.35, and the value of r where the potential crosses x-axis is about the same for all the potentials. The parameter values were selected to yield potentials where either the width, the depth or the product of width and depth was the same as for the unmodified potential. For all the modified potentials the lattice stability was tested by carrying out the simulation of thermal motion at 300 K, and comparing the radial density functions after the simulation. The repulsive potential used in the simulations was the DMol potential.

The simulations were carried out with the unmodified and six modified potentials. Parameters for the width and the depth of the potentials are given in table I. The width is defined as the full width at half minimum of the total potential, i.e. the potential where the repulsive part has been joined to the modified Stillinger-Weber potential.

The time evolution of the number of vacancies is shown in fig. 4. The statistical error of the number of vacancies is about 2 for all the potentials. During the first 100 fs the number of vacancies rises about equally for all the potentials. After this the results start to differ, reflecting the differences in the attractive potential. After about 500 fs an approximately stable value in the number of vacancies is reached. Simulations carried out with the

Potential	Width (Å)	Depth (eV)	Vacancies	Monovac.	Others
1. (unmodified)	0.903	2.16	27	15	8
2. (narrower)	0.847	2.16	16	12	4
3. (narrower, deeper)	0.847	2.28	19	13	6
4. (wider)	0.924	2.16	37	18	15
5. (wider, shallower)	0.924	2.10	36	19	12
6. (deeper)	0.903	2.28	32	15	12
7. (shallower)	0.903	2.10	23	13	7

Table I. Widths and depths for the unmodified and six modified Stillinger-Weber potentials. The average number of vacant sites, monovacancies and more complex vacancies produced in a collision cascade by one 300 eV Si atom recoiling in c-Si are shown in the three last columns.

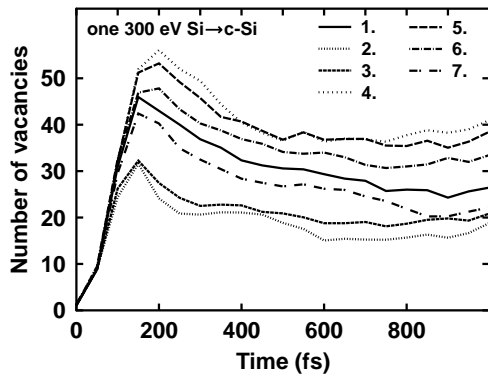


FIG. 4. Average number of vacancies produced during the first 1000 fs by one 300 eV Si atom for the 7 modified Stillinger-Weber potentials given in table I. The numbers are averages calculated from at least 30 simulation events.

For the unmodified Stillinger-Weber potential (potential 1) the number of vacancies (N_V) is 27. Potential 2 with the same depth and a 5% narrower width, results in a significantly smaller number of vacancies than potential 1, i.e. 16. Potential 3 which has the same width as potential 2 but where the depth has been modified so that the product of the width and depth is the same as for potential 1, yields about the same value of N_V as potential 2.

Potential 4 which has the same depth as potential 1 but a 2% wider width, leads to a clearly higher value of $N_V = 37$ than potential 1. Potential 5 with the same width as potential 4 and the same product of width and depth as potential 1, results in about the same number of vacancies as potential 4.

In potentials 6 and 7 the depth of the potential has been modified to the same values as for potentials 3 and 5, respectively, but the width is the same as for potential 1. The number of vacancies obtained differs somewhat from the values of the unmodified potential but the difference

is significantly smaller than for the potentials 2, 3, 4 and 5 where the width was changed.

The results indicate that the width of the potential has a strong effect on N_V . The behaviour can be understood qualitatively in terms of the interatomic forces. The width of the well reflects the strength of the forces involved when the bond is about to be broken. A narrower well means that the derivative of the potential, i.e. the force between the atoms, is stronger at the well borders resulting in stronger bonds and thus smaller numbers of vacancies.

Comparison of the potentials 3 and 5 with the potentials 2 and 4, respectively, and the potentials 6 and 7 with the potential 1 show that a deeper potential yields a somewhat higher number of vacancies, and vice versa. This somewhat surprising effect is significantly weaker than the effect of the width of the potential, however.

What is especially interesting is that relatively small changes in the potential result in large changes in N_V . For instance, a 2% increase in the width of the potential between the potentials 1 and 4 yields a 37% increase in N_V .

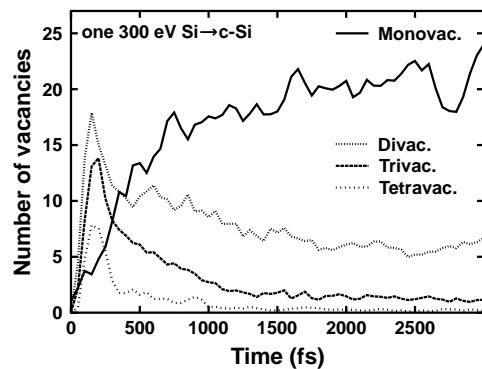


FIG. 5. Time evolution of the number of mono-, di- tri- and tetravacancies. The numbers are averages calculated over 10 events with the unmodified Stillinger-Weber potential.

The time evolution of different vacancy type defects is shown over a longer time scale in fig. 5. The number of pentavacancies is negligible and is therefore not shown. The number of complex (di-, tri-, and tetra-) vacancies increases rapidly in the beginning of the cascade, but decreases slowly after that, whereas the number of monovacancies increases steadily. This indicates that the complex vacancies slowly break down to monovacancies.

Because monovacancies are mobile in silicon at room temperature [22], they should disappear on a longer time scale, of the order of μ s or ms. Due to limitations in the available computer capacity, simulations of this process could not be carried out.

The Kinchin-Pease equation is generally used to estimate the number of vacancies produced in ion irradiations of solids. The total number of vacancies N_V produced during ion irradiation is

$$N_V = \frac{F_{D_n}}{2E_d} \quad (2)$$

where F_{D_n} is the deposited nuclear energy.

Values for the parameter E_d have been determined empirically by measuring the number of Frenkel pairs produced. The values of E_d given in the literature for silicon

range from about 15 to 25 eV, refs. [20,21]. The equation predicts that the number of Frenkel pairs (corresponding to the number of monovacancies in our simulations) produced by one 300-eV recoil should be below 10. Comparison of this value with the values for monovacancies in table I indicate that the unmodified Stillinger-Weber potential is not suitable for simulations of collision cascades. The numbers of vacancies obtained with the potentials with a narrower well are nearer the values predicted by the Kinchin-Pease equation.

4. CONCLUSIONS

In this work we demonstrated the need and feasibility to collect representative statistics when vacancy production in collision cascades due to ion irradiations is simulated in MD calculations. We showed that vacancy production is sensitive to the attractive potential but not to the repulsive potential. We obtained that the Stillinger-Weber potential suitable for the simulations of c-Si at or near equilibrium does not adequately describe interatomic interactions in collision cascades and that a modified potential with an at least 5% narrower well than that of the Stillinger-Weber potential results in a realistic description of vacancy production in classical MD simulations.

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