# Molecular dynamics calculation studies of interstitial-Si diffusion and arsenic ion implantation damage

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**Abstract – Silicon self-interstitial atom diffusion and implantation induced damage were studied by using molecular dynamics methods. The diffusion coefficient of interstitial silicon was calculated using molecular dynamics method based on the Stillinger-Weber potential. A comparison was made between the calculation method based on the Einstein relationship and the method based on a hopping analysis. For interstitial silicon diffusion, atomic site exchanges to the lattice atoms occur, and thus the total displacement-based calculation underestimates the ideal value of the diffusivity of the interstitial silicon. Through a study of molecular dynamics calculation for the arsenic ion implantation process, it was found that the damage self-recovering process depends on the extent of damage. That is , damage caused by a single large impact easily recovers itself. In contrast, the damage leaves significant defects when two large impacts in succession cause an overlapped damage region.**

## I. INTRODUCTION

Recent attempts to fabricate smaller ULSI devices and shallower junctions have created many challenging tasks in the area of process modeling. In addition to the conventional diffusion-reaction equation modeling, some atomistic simulations have proven to be practical for elucidating detailed mechanisms that can help us construct more accurate and efficient models. Molecular dynamics (MD) calculations have become capable of accurately simulating silicon-related processes since the Stillinger-Weber potential[1] was first proposed. This paper presents the results of molecular-dynamics studies for interstitial silicon diffusion, and for ion implantation damage produced by arsenic ions.

## II. CALCULATION METHOD

A calculation program was developed based on the molecular dynamics method with the Stillinger-Weber potential[1]. Computational efficiency was greatly improved ($\mathcal{O}(N^3) \rightarrow \mathcal{O}(N)$) by introducing a separable three-body potential form[2] and a block-search algorism that searches for atoms within a cut-off distance. Both NVE and NVT ensembles were used with Gear's scheme for the time integration. Typical calculation system sizes are $5 \times 5 \times 5$ silicon lattice unit cells (1001 atoms) for the interstitial diffusivity calculation, and $14 \times 14 \times 14$ lattice cells for the arsenic implantation simulation. The ZBL potential[9] was used for the arsenic-silicon interatomic potential. All the calculations were performed on an NEC EWS4800 (R10000) workstation and an NEC Cenju-4 parallel computer. Typical calculation times (CPU time) for the single workstation are 100-200 hours for calculating interstitial silicon diffusion for a period of 1-2 nano-seconds, and 4 seconds for one time step for ion implantation simulation where the time-step size is dependent on ion velocity.

## III. RESULTS AND DISCUSSION

### *Part 1: Interstitial-Si diffusivity calculation*

Our molecular dynamics calculation shows that the interstitial silicon atom (self-interstitial) equilibrium configuration is a $\langle 110 \rangle$ dumbbell site (Fig.1 or Fig.2) as well as described in Ref.[3]. We have also checked this configuration by higher order calculation methods, such as tight-binding molecular dynamics calculation[5][6] and ab initio calculation based on the density functional theory with local density approximation (LDA). Stillinger-Weber potential gives a slightly different configuration for the most stable interstitial silicon $\langle 110 \rangle$ dumbbell structure as shown in Fig.2. However, the formation energy of the interstitial silicon calculated as 3.7 eV by the Stillinger-Weber potential, is comparable to the 3.5-3.8 eV of the tight-binding model[6] or the 3.3 eV of the LDA results[7]. Therefore, the following studies were performed via molecular dynamics calculation based on the Stillinger-Weber potential.

In [3] and other previous calculations of the diffusivity were based on the Einstein relationship where all the individual atom displacement (actually their square-value) amounts were accumulated over a sufficient time period. This method, however, implicitly overfeeds the interstitial-Si displacement due to the thermal-vibration of lattice atoms. Moreover, the self-interstitial migration picture must account for exchanges between the interstitial-atom and lattice atoms, and thus its diffusivity must be an *effective* quantity. However, the total-displacement based method overlooks this exchange, since the square-displacement values for each individual atom are accumulated regardless of which atoms are interstitial-atoms.

In our calculation, the self-interstitial location was directly determined by monitoring atomic potential values to account for exchanging with lattice atoms. The diffusion constant for the interstitial-Si was calculated by analyzing its hopping motions

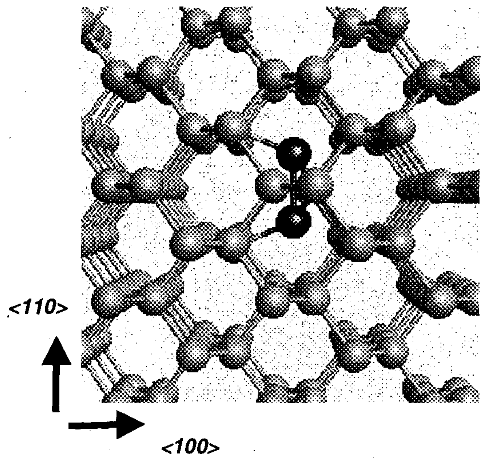

Figure 1: Equilibrium configuration of the interstitial silicon obtained by the molecular dynamics calculation of the annealing after adding one extra atom to a perfect lattice system. This dumbbell-like structure along the $\langle 110 \rangle$ axis is the most stable interstitial silicon atomic configuration predicted by tight-binding molecular dynamics calculation. The formation energy is calculated as 3.9 eV by using tight-binding molecular dynamics (216+1 atom unit-cell).

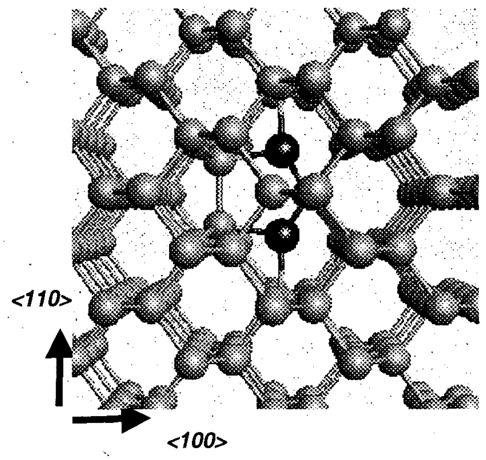

Figure 2: The most stable configuration of interstitial silicon with the Stillinger-Weber (SW) potential. The dumbbell-like structure is almost the same as that in Fig.1, with slight distortion of the two nearest silicon lattice atoms. Formation energy is calculated as 3.7 eV by using the SW potential MD.

among equilibrium sites ($\langle 110 \rangle$dumbbell). Figure 3 shows one of the calculation results for tracing self-interstitial migration in the silicon lattice. Average hopping time ($\tau$) and distance ($L$) can be read from the steps of the coordinate plot lines in Fig.3, after which they were compiled to the self-interstitial diffusivity ($D_I = L^2/6\tau$).

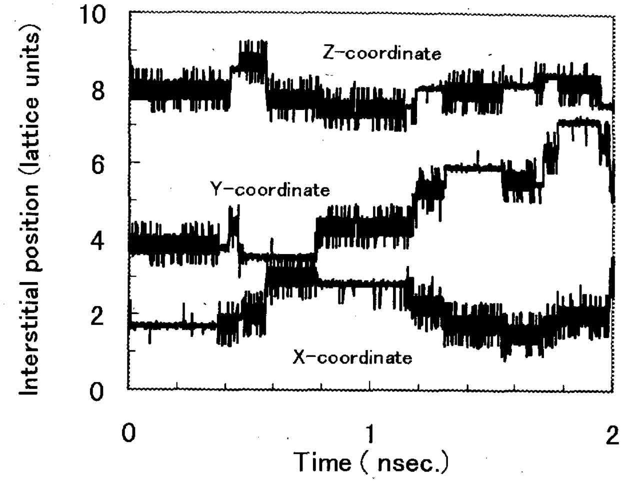

Figure 3: Calculation result for self-interstitial migration in the silicon lattice at 1073 Kelvin, up to 2 nano-seconds.

Table 1: Molecular dynamics calculation results by using Stillinger-Weber potential, for the hopping analysis.

| Temperature | 1073K | 1173K | 1273K |
|---|---|---|---|
| Time period | 2.0 nsec. | 1.0 nsec. | 1.0 nsec. |
| Number of hops | 11 | 12 | 23 |
| Hop distance(nm) | 0.543 | 0.543 | 0.543 |
| Hop interval(nsec.) | 0.182 | 0.08833 | 0.0435 |

A comparison was made between this hopping analysis and the method based on the Einstein relationship (i.e., the sum of all the atom displacements). In order to calculate the self-interstitial diffusivity for the Einstein relationship based method, some of the displacements due to the thermal-vibration must be deducted from the sum of all the atom displacements (See Fig.4).

Figure 5 shows the calculation results for the self-interstitial diffusivity using these methods. As the figure shows, the diffusivity values decrease from the values represented by the plots denoted (in a) to the values represented by the plots (b).

Our hopping analysis leads to equation 1. The activation energy of 0.89 eV is comparable to other recently obtained values. [3][8].

$$D_I = 0.039 \exp(-0.89/kT)[cm^2/sec] \qquad (1)$$

In interstitial silicon diffusion, atomic exchange occurs between the interstitial atom and lattice atoms during the hopping

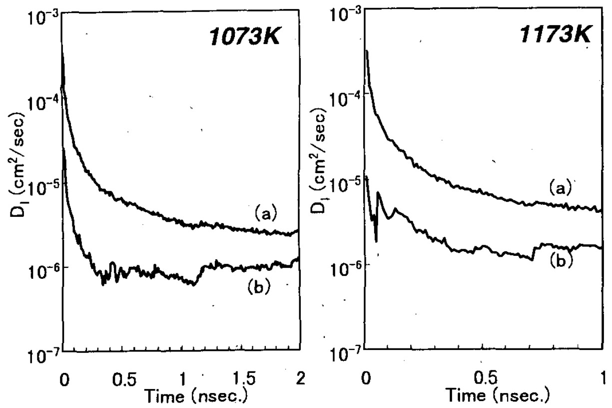

Figure 4: Calculation result for self-interstitial diffusivity from the Einstein relationship, i.e. (a) $D_I = \sum(x - x_0)^2/6t$. (b) Small displacements due to the thermal vibration of lattice atoms, was deducted from (a).

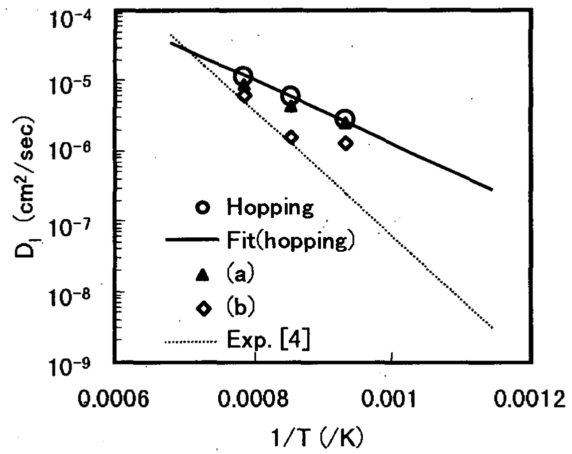

Figure 5: Calculation results for the self-interstitial diffusivity. Open circles: Hopping analysis. (a) Calculated values based on total displacement of all atoms. (b) Deducted small displacements due to thermal vibration of lattice atoms from (a).

motion. Therefore, total displacement based calculation underestimates the ideal value of interstitial-Si diffusivity. Hopping analysis can trace interstitial silicon motion when temperatures are not very high ( <1100℃). The interstitial migration can hardly be considered as discrete hopping motion for such a high temperature.

*Part 2: Arsenic ion implantation simulation*

For arsenic ion implantation, the large impact of this heavy ion on the silicon crystal lattice causes significant smashing damage to the crystalline structure. Through MD simulation, it was found that self-recovery from this smashing damage depends on the extent of the damage. Figure 6 shows the MD simulation results for a single arsenic ion implantation into the ideal silicon lattices. It was found that the damage caused by a single large impact is easily recovered from. In contrast, the damage leaves significant defects when two succeeding large impacts cause an overlapped damage region, as shown in Fig.6(b).

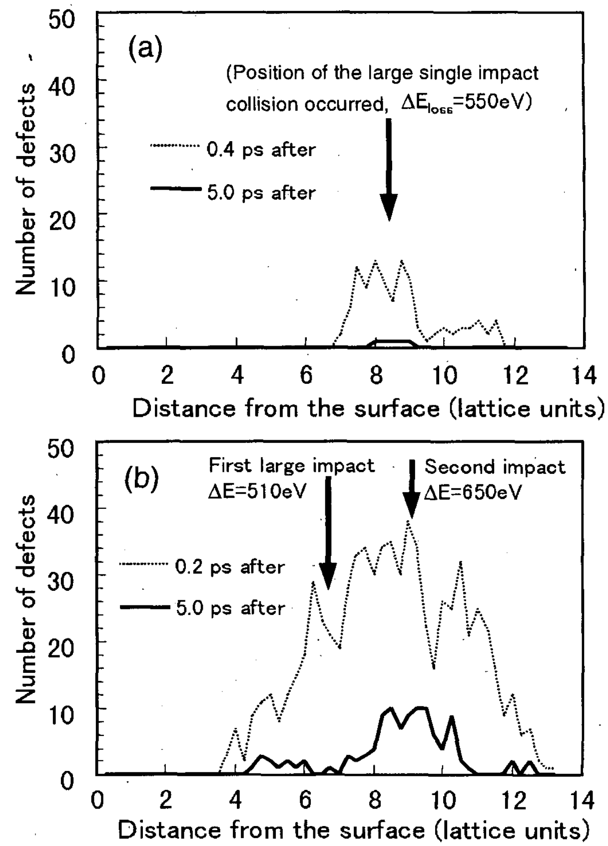

Figure 6: Calculation results for the number of defects created by large incident arsenic ion impact collisions. (a) Only a single large impact: the smashing damage was almost completely recovered from after 5 ps. Effective displacement threshold energy $E_D$ = 129.4eV. (b) Two large impact events occurred close to each other: significant number of defects remains. In this case, $E_D$ = 12.8eV.

We can conclude, therefore, that conventional Monte Carlo simulation[10] seems to underestimate dechanneling effects for the passing ions, since the threshold energy for the damage creation is usually constant and independent of the lattice damage.

For modeling a very low energy arsenic implantation, the

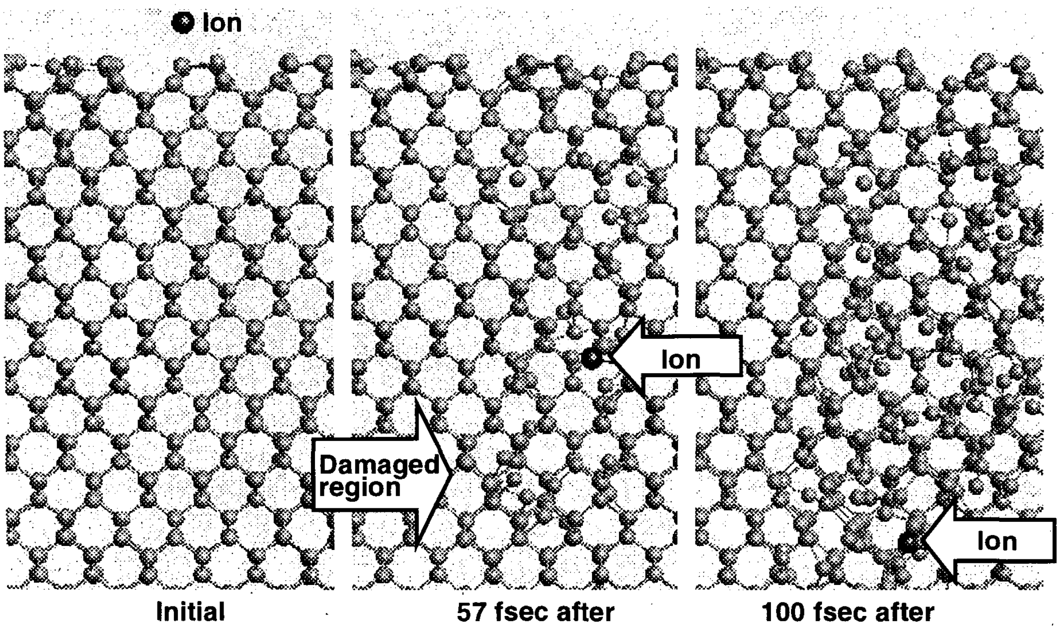

Figure 7: 3 keV arsenic ion implantation simulation results. Recoiled silicon atoms became faster than the arsenic ion. It can be observed that the arsenic ion passes through the temporarily damaged region produced by the faster recoiled silicon atoms.

damage creation process and the resulting de-channeling process must be considered in a more accurate way. Despite the fact that the implantation energy is low, recoiled silicon atoms become much faster than the implanted arsenic ion itself since an arsenic atom is much heavier than a silicon atom. Therefore, heavy damage is temporarily created prior to the arsenic ion passing, then self-recovers after the ion passing. Figure 7 shows the simulation results for 3 keV arsenic ion implantation into a (100) silicon surface. It can be observed that the arsenic ion passes through the temporarily damaged region produced by the faster recoiled silicon atoms, meaning that the ion suffers hardly some of the channeling effect that would have occurred if it were assumed that the implanted ion did not create any damage.

## IV. SUMMARY

Molecular dynamics studies on point defects and ion implantation provided a detailed picture of the atomic diffusion and the transient behavior of defects created during ion implantation processes. The information thus obtained can be effectively utilized for improving conventional process simulation models.

## ACKNOWLEDGMENT

The authors would like to thank Dr. O. Sugino and Dr. Y. Miyamoto of NEC Fundamental Research Laboratories, for providing tight-binding model and LDA programs, and for their useful comments and discussions.

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