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Molecular Dynamics Simulation for Focused Ion Beam processing: A comparison between computational domain and potential energy

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Abstract. Molecular dynamics calculation was performed to simulate nano-Focused Ion Beam (FIB) processing on a Silicon surface. A combination of potential functions of impacting ion and target atoms was evaluated, and the influence of computational domain along the lateral directions was estimated. The target Silicon atoms on (100) surface of Si crystal were described by Tersoff potential. Ion-beam source was represented by Ga ions, where the optimal potential of the Ga ion was chosen by comparing Lennard-Jones, Tersoff, and ZBL (Ziegler, Biersack and Littmark) potentials. The initial velocity of ion was 3.327×10⁵ m/sec at 40 keV.

First, for the evaluation of combined potential functions of Si atoms and Ga ion, a small computation volume (2.58 nm × 2.58 nm × 51.99 nm) consisting of 19200 Si atoms was chosen with a single Ga ion impacting on Si (100) surface. On the combination of Tersoff potential for Si atom, and ZBL potential for Ga ion, the depth of the combination was found to be in good agreement with the depth of SRIM. Next, the influences of computational domain in lateral direction were evaluated by a larger region with a combination of potentials where the computational volume was (8.55 nm × 8.55 nm × 51.99 nm) constructed by 196608 Si atoms. Consequently, the energy transfer along lateral computational length was faster in larger region than in smaller region, and the entire initial energy of Ga ion was transmitted to the target material.

1. Introduction
Focused ion beam (FIB) is a very attractive tool in lithography [1], doping [2], deposition [3], and etching [4]. In particular, FIB etching and deposition techniques have been widely used for mask repair [5] and for sample preparation for transmission electron microscope[6]. Recently, these techniques have been extended toward the fabrication of three-dimensional (3D) nanostructure. FIB-chemical vapor deposition (CVD) is used to fabricate 3D nanostructure, and to aerial wiring which are applied to photonic crystal and nano-scale tweezers [7,8]. On the other hand, FIB etching has had very limited use in the fabrication and formation of 3D structure such as predetermined curved shape, microlens components, and diffractive optical elements [9,10], because of their very demanding specification on etching tasks. Usually, FIB etching is estimated by employing sputtering formula derived by Sigmund [11]. However, behaviors of implanted ions, collisions among ions and atoms in
lattice, and sputtered atoms cannot be tracked dynamically. Therefore, understanding of FIB etching at atomic scale becomes important for the fabrication of 3D nanostructure. In order to understand the phenomena of etching by ions into solid substrate, molecular dynamics simulation is a powerful method, because it can track each ion and atom dynamically. In this paper, molecular dynamics simulations were carried out that led to the findings of optimal potential function by small- and large-scale computational domains. The influence of lateral computational domain is shown for the computational result.

2. Simulation method
We performed molecular dynamics simulations with two computational regions. One was to find out optimal combination of potential functions for target material and impacting ion, and the other was to investigate the influence of lateral computational region for the computational result via large-scale molecular dynamics (MD) simulation. In the present MD calculations, the Verlet algorithm was used for time integration.

2.1. Potential function for Si crystal
For all simulation of the target material Si, Tersoff potential function [12] was employed.

\[
\phi = \frac{1}{2} \sum_i \sum_{j \neq i} f_c (r_{ij}) \left\{ f_R (r_{ij}) + b_j f_A (r_{ij}) \right\}
\]

\[
f_R (r) = A \exp (-\lambda r) \quad f_A (r) = \begin{cases} 1, & r < R \\ \frac{1}{2} + \frac{1}{2} \cos \frac{\pi (r - R)}{S - R}, & R < r < S \\ 0, & r > S \end{cases}
\]

\[
b_j = \left( 1 + \beta^n \zeta^n \right)^{-1/2n}, \quad \zeta_j = \sum_{k \neq i, j} f_c (r_{ik}) g (\theta_{ijk}), \quad g (\theta) = 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (h - \cos \theta)^2}
\]

Here \( i, j, \) and \( k \) label the atoms of the system, \( r_{ij} \) is the length of the \( ij \) bond, and \( \theta_{ijk} \) is the bond angle between bounds \( ij \) and \( jk \). The parameters in Eq. (1) are summarized in Table 1. When Ga ion is represented as Tersoff potential function [13], those parameters are also expressed in Table 1.

| \( A [\text{eV}] \) | \( 1.8308 \times 10^3 \) | \( 2.83982 \times 10^3 \) |
| \( B [\text{eV}] \) | \( 4.7118 \times 10^2 \) | \( 1.14786 \times 10^2 \) |
| \( \lambda_1 [\text{Å}^{-1}] \) | \( 2.47999 \) | \( 3.2834 \) |
| \( \lambda_2 [\text{Å}^{-1}] \) | \( 1.7322 \) | \( 1.7154 \) |
| \( n \) | \( 7.8734 \times 10^{-4} \) | \( 3.4729 \) |
| \( \beta \) | \( 1.1000 \times 10^6 \) | \( 2.3586 \times 10^4 \) |
| \( c \) | \( 1.0039 \times 10^5 \) | \( 7.6028 \times 10^2 \) |
| \( d \) | \( 1.6217 \times 10^4 \) | \( 1.9796 \times 10^4 \) |
| \( h \) | \( -5.9825 \times 10^1 \) | \( 7.1459 \times 10^1 \) |
| \( R [\text{Å}] \) | \( 2.7 \) | \( 2.8 \) |
| \( S [\text{Å}] \) | \( 3.0 \) | \( 3.0 \) |

2. Simulation method

| \( \sigma [\text{Å}] \) | \( 2.485 \) |
| \( \varepsilon [\text{eV}] \) | \( 8.075 \times 10^3 \) |

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| \( c_i \) | \( d_i \) |
| \( 1 \) | \( 0.028171 \) | \( 0.20162 \) |
| \( 2 \) | \( 0.28022 \) | \( 0.40290 \) |
| \( 3 \) | \( 0.50986 \) | \( 0.94299 \) |
| \( 4 \) | \( 0.18175 \) | \( 3.1998 \) |
Moreover, Si-Ga interaction parameters are calculated using the following arithmetic and geometric means:

\[
A = \sqrt{A_A A_B}, \quad B = \sqrt{B_A B_B}, \quad R = \sqrt{R_A R_B}, \quad S = \sqrt{S_A S_B}
\]

\[
\lambda = (\lambda_A + \lambda_B) / 2, \quad \mu = (\mu_A + \mu_B) / 2
\]

2.2. Lennard-Jones potential for Ga ion

One of calculations employed Lennard-Jones potential function to represent Ga ion as shown here:

\[
\phi(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^12 - \left( \frac{\sigma}{r_{ij}} \right)^6 \right]
\]

Here the potential is fitted with the diameter of Ga atom, and \(\varepsilon\) is determined by the proportion of values based on rare gas. The parameters are shown in Table 2.

2.3. Ga ion for Ziegler, Biersack and Littmark (ZBL) potential

Ga ion potential is represented by ZBL (Ziegler, Biersack and Littmark) potential [14].

\[
\phi(r) = \frac{Z_1Z_2\sigma^2}{4\pi\varepsilon r_{ij}} \Phi(r)
\]

\[
\Phi(r) = \sum_{k=1}^{4} c_k \exp \left( -d_k \frac{r_{ij}}{a_0} \right), \quad a_u = \frac{0.8854a_u}{Z_j^{0.23} + Z_j^{0.23}}, \quad a_0 = 0.529\text{Å}
\]

Where \(Z_1, Z_2\) are atomic numbers. The detail parameters are shown in Table 3.

3. Computational parameters

3.1. Small-scale simulations for computational parameters

Figure 1 shows a computational domain for small-scale calculation.
The target domain is 2.58nm × 2.58nm × 51.99 nm, which is constructed by 19200 Si atoms, and also represents single Ga ion impact on Si (100). The x- and y-directions are adapted to the periodic boundary conditions. Top boundary represents free boundary condition, and bottom boundary is a fixed heating bath layer. Three cases in Table 4 are considered to find the optimal combination of potential functions for Si and Ga.

### Table 4. Parameter for Ga ion.

| Case   | Ga-Si      | Si-Si      | Computational region       |
|--------|------------|------------|----------------------------|
| Case A | Tersoff    | Tersoff    | 2.58 nm × 2.58 nm × 51.99 nm |
| Case B | Lennard-Jones | Tersoff    | 2.58 nm × 2.58 nm × 51.99 nm |
| Case C | ZBL        | Tersoff    | 2.58 nm × 2.58 nm × 51.99 nm |
| Case D | Tersoff    | Tersoff    | 8.55 nm × 8.55 nm × 51.99 nm |
| Case E | Lennard-Jones | Tersoff    | 8.55 nm × 8.55 nm × 51.99 nm |
| Case F | ZBL        | Tersoff    | 8.55 nm × 8.55 nm × 51.99 nm |

3.2. Large-scale simulations for computational parameter

Computational domain for large-scale calculation is shown in Fig. 2. The target domain is 8.55 nm × 8.55nm × 51.99 nm, which is constructed by 282752 Si atoms. The x- and y-directions are also adapted to the periodic boundary conditions. Top boundary represents a free boundary condition, and bottom boundary is fixed heating bath layer. Three cases in Table 4 are considered to investigate the influence of lateral computational domain.

4. Result and Discussion

Figure 3 shows the depth versus time developing for six cases. The profile for Case A is linear and presented by a straight line. It shows a velocity approximately equal to $3.327 \times 10^5$ m/sec, which is calculated by the gradient of the linear profile. Thus, it is evident that no energy transfer took place since the initial velocity of ion was also $3.327 \times 10^5$ m/sec. For Case B, the depth value saturate at 60 [fsec], and is smaller than SRIM value. For Case C, the depth value saturate at 70 [fsec], and is larger than SRIM value. The depth is overestimated because the computational region along x- and y-directions is narrow. It is necessary that the computational region at x- and y-directions be significantly wide. When Tersoff potential is used, energy is not transmitted to the sample regardless of the calculation area. When it uses the Lennard-Jones potential, it doesn't change, and the penetration into its depth is shallower than SRIM regardless of the calculation area.

![Figure 3. Depth profile.](image-url)
Figure 4. Energy distributions for each division:
(a) Case A, (b) Case B, (c) Case C, (d) Case D, (e) Case E, (f) Case F.

Figure 4 shows energy distribution for the six cases. The distribution profiles show how the collision energy is transmitted from surface to the bottom area. Thus, each line in the figures is averaged energy distribution for the parallel partitions from surface to the bottom on the target Silicon material, and where the target volume is divided into 16 partitions. Note that the energy profile is enhanced from the surface to the growing bottom one by one, and the speed spread at the bottom can be understood because a horizontal axis represents time in the figure. For Case A and Case D, the energy is not transferred to the target, and the value is almost zero. This indicated that Ga ion impact energy cannot be transferred using Tersoff potential for Ga ion.
For Case B and Case E, the energy transfer to the target and the profiles are almost same. This phenomenon shows same tendency toward the depth profiles (see Fig. 3). For Case C and Case F, both the energy transfer profiles are very well, however, in Case F with larger computational region, the energy is enhanced on faster time and the value is higher and is close to the initial ion energy. Thus, in case of larger computational domain at lateral directions, the collision process is accurately expressed.

5. Conclusions
Large- and small-scales molecular dynamics simulations were carried out to understand the influence of the potential combination of ion and target material and the influence of lateral computational domain. The potential combination is found for Silicon and Ga ion: Silicon is Tersoff potential, and Ga ion is ZBL potential. From the knowledge of small-scale simulation, it is important to define widely the computational region along x- and y-directions to indicate the depth being comparable to previous value such as SRIM. In comparison with large- and small-scale simulations, the computational region along x- and y-direction is significant since here the different sputtering mechanisms were found using small computational domain. Thus, in case of small computational domain, the sputtering atoms achieved to the x- and y-boundary directions, and the energy spread to lateral directions. Therefore, the collision energy cannot be accurately transferred in the z-direction.

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