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An interatomic potential model for molecular dynamics simulation of silicon etching by Br⁺-containing plasmas

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An interatomic potential model for Si–Br systems has been developed for performing classical molecular dynamics (MD) simulations. This model enables us to simulate atomic-scale reaction dynamics during Si etching processes by Br⁺-containing plasmas such as HBr and Br₂ plasmas, which are frequently utilized in state-of-the-art techniques for the fabrication of semiconductor devices. Our potential form is based on the well-known Stillinger–Weber potential function, and the model parameters were systematically determined from a database of potential energies obtained from ab initio quantum-chemical calculations using GAUSSIAN03. For parameter fitting, we propose an improved linear scheme that does not require any complicated nonlinear fitting as that in previous studies [H. Ohta and S. Hamaguchi, J. Chem. Phys. 115, 6679 (2001)]. In this paper, we present the potential derivation and simulation results of bombardment of a Si(100) surface using a monoenergetic Br⁺ beam. © 2008 American Institute of Physics. [DOI: 10.1063/1.2990070]

I. INTRODUCTION

Understanding the interaction between chemical plasmas and material surfaces is of utmost importance when fabricating semiconductor devices. Recently, process sizes of device structures in the large-scale integration chips have reached a deep submicron level less than 50 nm. Therefore, a thorough (i.e., at the atomic-scale level) understanding via numerical simulations is necessary.

During plasma processing, high-energy ions (typically 10–500 eV) accelerated in the plasma sheath are injected into the material surface. In this case, a very large number of simulation particles are required for the dynamic simulation of reaction processes. Therefore, classical molecular dynamics (MD) simulation using a preconstructed interatomic potential model is very useful because the low simulation cost involved facilitates a systematic parameter survey.

The construction of a potential model is vital for performing classical MD simulations. Herein, we summarize the potential models developed for plasma etching simulations. Stillinger and Weber (SW) developed a potential model with two-body and three-body functions for Si and F systems.1,2 These potential functions are designed to reproduce some of the structural and thermodynamic characteristics of the materials and the relevant structural chemistry for some selected molecules comprising these elements. Feil et al.3 also applied this function form to Si and Cl systems by determining new parameter sets. Weakliem et al.4 have modified the original SW potentials for Si–F systems using the interatomic potential data obtained from ab initio quantum-chemical calculations for performing MD simulations of fluorine adsorption on silicon. Hanson et al.5 have also modified Feil’s model for Si–Cl systems by adding new terms, i.e., an embedding term and a four-body term based on the ab initio data, in order to represent a highly realistic surface reaction during plasma etching including low-energy neutral radicals. Ohta et al.6 developed two sets of potential models for Si–O–F and Si–O–Cl systems based on previously reported potential models for Si–F, Si–Cl, and Si–O systems with additional ab initio data. Here, the models for Si–O systems were originally developed by Watanabe et al.7 for a large-scale modeling of SiO₂/Si interface structures. Further, a potential model with multibody interactions based on bond-order potential was developed by Tersoff,8–10 and the parameters for Si, C, and Si–C systems have been currently made accessible. These potential models were extended to C–H systems by Brenner11,12 in order to study various small hydrocarbon molecules as well as graphite and diamond lattices. Tanaka et al.13 and Abrams et al.14 also determined parameter sets for C–F and C–Si–F systems based on Brenner’s empirical models in order to perform MD simulations of surface reactions caused by fluorocarbon plasmas. Most recently, potential models for Si–O–C–F systems for performing MD simulations of SiO₂ etching by fluorocarbon plasmas were reported by Ohta and Hamaguchi,15 Ohta,16 and Smirnov et al.17 The latter is based on SW-type potential functions.17 In addition, Smirnov et al.18 further extended the SW models to Si–O–C–H systems for plasma etching simulations of low-k dielectric materials. Finally, interactions between Ar and other elements can be described by using Morièré repulsive pair potentials.19

Generally, since halogens show strong chemical reactivity toward Si surfaces, F⁺-or Cl⁺-containing plasmas have been used for Si etching processes. With the etching process being reduced up to the deep submicron scale, Br⁺-containing plasmas such as HBr and Br₂ plasmas have been introduced in the actual manufacturing process. There are several published reports on fundamental experiments on the same.20–22 On the contrary, no potential models contain-
ing Br have been developed, although they are very important in state-of-the-art dry-process techniques.

In this study, we present a procedure for developing a potential model for Si–Br systems based on the well-established SW-type potential. The model parameters are determined entirely from ab initio quantum-chemical calculations for small clusters. Herein, we also report a detailed procedure for determining the model parameters and sample simulations of Si etching by a monoenergetic Br⁺ beam.

II. SW-TYPE POTENTIAL FUNCTIONS

First, the SW-type potential model for covalent bonds is summarized.1–3,6 The total energy of an atomic system is determined entirely from quantum-chemical calculations.1–3 In state-of-the-art dry-process techniques.

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\[
\Phi = \sum_{i<j} v_2(i,j) + \sum_{i<j<k} v_3(i,j,k).
\]

The total energy of an atomic system is determined entirely from quantum-chemical calculations.1–3

\[
v_2(i,j) = \frac{C_{ij}}{r_{ij} - a_{ij}} \exp \left( \frac{r_{ij} - a_{ij}}{C_{ij}} \right)
\]

and

\[
v_3(i,j,k) = v_3(r_{ijk}) = h_{ijk}(r_{ijk}, r_{ik}, r_{jk}, \theta_{ijk})
\]

where \( \theta_{ijk} \) is the angle spanned by \( r_{ij}, r_{jk}, \) and \( r_{ik} \), and \( h_{ijk} \) is given by either

\[
h_{ijk}(r_{ijk}, \theta_{ijk}) = \begin{cases} 
\frac{\gamma_{ijk}}{r - a_{ijk}^1} + \frac{\gamma_{ijk}^2}{s - a_{ijk}^2} & \text{if } r < a_{ijk}^1 \text{ and } s < a_{ijk}^2 \\
0 & \text{otherwise,} \end{cases}
\]

or

\[
h_{ijk}(r_{ijk}, \theta_{ijk}) = \begin{cases} 
\frac{\gamma_{ijk}^1}{r - a_{ijk}^1} + \frac{\gamma_{ijk}^2}{s - a_{ijk}^2} & \text{if } r < a_{ijk}^1 \text{ and } s < a_{ijk}^2 \\
0 & \text{otherwise,} \end{cases}
\]

depending on the species of the (i,k) atom if \( r < a_{ijk}^1 \) and \( s < a_{ijk}^2 \), otherwise, \( h_{ijk} = 0 \). Here, \( \lambda_{ijk}, \gamma_{ijk}, \gamma_{ijk}^1, \gamma_{ijk}^2, a_{ijk}^1, a_{ijk}^2, \theta_{ijk}, \) and \( \alpha_{ijk} \) are parameters that depend on the species of the (i,k) triplet. \( a_{ijk}^1 \) and \( a_{ijk}^2 \) are the cutoff distances. The system symmetry requires these parameters to be invariant when the first and third indices in the subscripts are exchanged, e.g., \( \lambda_{ijk} = \lambda_{kij}, \gamma_{ijk} = \gamma_{kij}, \gamma_{ijk}^1 = \gamma_{kij}^1, \) and \( \gamma_{ijk}^2 = \gamma_{kij}^2 \).

We have added a new parameter \( a_{ijk} \) in order to improve parameter fitting to the level achieved in previous studies.7

III. PARAMETER FITTING PROCEDURE

A. Quantum-chemical calculations by GAUSSIAN03

Let us introduce two assumptions for the systems studied herein. First, we consider atomic interactions only among charge-neutral species. In other words, isolated clusters such as atoms, molecules, radicals, and the surface itself are maintained neutral. Then, we impose the adiabatic assumption for electron dynamics (Born–Oppenheimer approximation) on the system. Then, the interatomic forces can be obtained from the derivatives of such interatomic potential functions with respect to the position of the nucleus.

For quantum-chemical calculations, we used the general-purpose software “GAUSSIAN03.”23 A density-functional method “B3LYP/6-311+G(d,p)” was adopted as the model chemistry and basis set because our systems contain 35Br whose atomic number is very high. Although the total charge of the input parameters is always zero since a charge-neutral condition is assumed, the total spin multiplicity \( S \) (number of lone pair electrons + 1) for each atomic configuration should be specified. The total potential energies calculated for various configurations of small clusters, i.e., the ab initio database, were used to determine the interatomic potential functions.

Determination of the parameters involves the following three steps: (1) determination of the two-body functions \( (v_{SBBr} \text{ and } v_{SBSi}) \), (2) determination of the three-body potential given by Eq. (3) \( (h_{SBBrB}, h_{SBBrSi}, \text{ and } h_{SBSiB}) \), and (3) determination of the three-body potential given by Eq. (4) \( (h_{SBBrB}, h_{SBBrSi}, \text{ and } h_{SBSiB}) \). The energy and length units in our potential functions (parameters) are 50.0 kcal/mol (2.17 eV) and 2.0951 Å, respectively.

B. Two-body functions

First, we determine the parameters for \( v_{SBBr} \) and \( v_{SBSi} \) for the Br–Br and Si–Br pairs, respectively. The ab initio data were obtained from calculations carried out for the Br–Br cluster \((S=1)\) and Si–Br cluster \((S=2)\) by varying the bond lengths. When the interatomic distance increases, the potential energy values may be overestimated because of the difficulty involved in the accurate calculation of the potential energies for open-shell structures. Hence, we excluded the data that exceeded a reference value.

For the Br–Br pair, the zero reference is considered to be twice the potential energy of an isolated Br atom \((S=2)\). Similarly, the zero reference for the Si–Br pair is the sum of potential energies of an isolated Si atom \((S=3)\) and a Br atom \((S=2)\). The ab initio data and potential curves with optimized fitting parameters are shown in Fig. 1. For \( v_{SBSi} \), we use the original SW parameters without further modification.6 The optimized parameters \( A_{ij}, B_{ij}, C_{ij}, p_{ij}, q_{ij}, \) and \( a_{ij} \) are summarized in Table I. The bond energies and bond lengths calculated by using two-body potential functions are 2.06 eV and 2.34 Å for the Br–Br bond and 3.67 eV and 2.32 Å for the Si–Br bond, respectively (see Table II).

...
C. Three-body functions [Eq. (3)]

Next, we determine three-body functions for $h_{\text{BrBrBr}}$, $h_{\text{BrBrSi}}$, and $h_{\text{SiBrSi}}$ using the potential function shown in Eq. (3). This function effectively introduces a single valence of a halogen atom by shielding the attractive forces arising from a simple summation of the two-body potentials. Here, we present the method of determination of the fitting parameters for $h_{\text{BrBrBr}}$. The same procedure was applied to the cases of $h_{\text{BrBrSi}}$ and $h_{\text{SiBrSi}}$. Note that the two-body potentials determined in the previous subsection are used here.

The function provided by Eq. (3) contains five parameters $\lambda_{ijk}$, $\gamma_{ijk}$, $\gamma_{ijk}^k$, $\lambda_{ijk}^k$, and $\lambda_{ijk}^k$. On the basis of our preliminary examination (not presented in this paper), we determined the values of $\lambda_{ijk}$ and $\gamma_{ijk}^k$ as follows: $\gamma_{ijk}^k = \gamma_{ijk}^k = \gamma_{ijk}^k = \gamma_{ijk}^k$. As a result, the conditions $\gamma_{\text{BrBrBr}} = C_{\text{BrBrBr}}$, $\gamma_{\text{BrBrSi}} = C_{\text{BrBrSi}}$, and $\gamma_{\text{SiBrSi}} = C_{\text{SiBrSi}}$ were satisfied. The remaining parameter $\lambda_{ijk}$ (in this case, $\lambda_{\text{BrBr}}$) should be optimized by considering all the two- and three-body functions for clusters that contain three atoms. The $ab\ initio$ data used here were obtained from the calculations performed for the Br–Br–Br ($S=2$) cluster by varying the bond lengths, with $h_{\text{BrBrBr}} = 180^\circ$, where the zero reference is thrice the potential energy of an isolated Br atom ($S=2$). Figure 2 shows the two-dimensional potential energy contours calculated using the complete potential model. In this figure, the small numbers indicate the potential energies (eV) corresponding to each contour. The definitions of $r_1$ and $r_2$ are provided at the top of the figure. The extracted one-dimensional potential curves are also shown. As shown here, the obtained potential curves are consistent with the $ab\ initio$ data although only $\lambda_{ijk}$ was determined as an independent parameter.

Similarly, the parameters for $h_{\text{BrBrSi}}$ and $h_{\text{SiBrSi}}$ are determined. Following the abovementioned procedure, we get $\gamma_{\text{BrBrSi}} = C_{\text{BrBrSi}}$, $\gamma_{\text{BrSiBr}} = C_{\text{BrSiBr}}$, $\gamma_{\text{SiBrSi}} = C_{\text{SiBrSi}}$, and $\gamma_{\text{SiSiSi}} = C_{\text{SiSiSi}}$ for $h_{\text{BrBrSi}}$. We obtained the relations $\gamma_{\text{SiBrSi}} = C_{\text{SiBrSi}}$, and $\gamma_{\text{SiSiSi}} = C_{\text{SiSiSi}}$ for $h_{\text{SiBrSi}}$. We determined separately the $ab\ initio$ data for the determination of $h_{\text{BrBrSi}}$ and $h_{\text{SiBrSi}}$. The obtained potential curves are consistent with the $ab\ initio$ data although only $\lambda_{ijk}$ was determined as an independent parameter.

As shown here, the obtained potential curves are consistent with the $ab\ initio$ data although only $\lambda_{ijk}$ was determined as an independent parameter.

Finally, the parameters for $h_{\text{BrBrSi}}$ and $h_{\text{SiBrSi}}$ are determined. Following the abovementioned procedure, we get $\gamma_{\text{BrBrSi}} = C_{\text{BrBrSi}}$, $\gamma_{\text{BrSiBr}} = C_{\text{BrSiBr}}$, $\gamma_{\text{SiBrSi}} = C_{\text{SiBrSi}}$, and $\gamma_{\text{SiSiSi}} = C_{\text{SiSiSi}}$ for $h_{\text{BrBrSi}}$. We obtained the relations $\gamma_{\text{SiBrSi}} = C_{\text{SiBrSi}}$, and $\gamma_{\text{SiSiSi}} = C_{\text{SiSiSi}}$ for $h_{\text{SiBrSi}}$.
(S=4), respectively. For these calculations, the bond lengths were used as the scanning parameters, and the three atoms were aligned in a linear fashion. The zero reference values were calculated by the appropriate summation of the potential energies of the Si atom (S=3) and Br atom (S=2). A comparison of the potential energies between GAUSSIAN03 and our model is shown in Figs. 3 and 4. As shown in these figures, our potential functions could reconstruct the ab initio data perfectly. Note that this procedure presented here does not require nonlinear fitting, in contrast to that reported in the previous studies; further, only $\lambda_{ijk}$ is considered as the independent parameter. All the parameters determined here are summarized in Table I.

D. Three-body functions [Eq. (4)]

Finally, the parameters for the three-body functions given by Eq. (4) were determined for $h_{BrSiBr}$ and $h_{BrSiSi}$. For these, we used the conditions mentioned in the previous subsection, i.e., $a_{BrSiBr} = \gamma_{BrSiBr} = C_{SiBr}$, $a_{BrSiSi} = \gamma_{BrSiSi} = C_{SiSi}$, $a_{BrSiBr} = \gamma_{BrSiBr} = C_{SiBr}$, and $a_{BrSiSi} = \gamma_{BrSiSi} = C_{SiSi}$. The remaining parameter sets are $(\lambda_{BrSiBr}, \theta_{BrSiBr}, \alpha_{BrSiBr})$ and $(\lambda_{BrSiSi}, \theta_{BrSiSi}, \alpha_{BrSiSi})$ for $h_{BrSiBr}$ and $h_{BrSiSi}$, respectively. The parameter sets for $h_{BrSiBr}$ and $h_{BrSiSi}$ were determined separately. We optimized the three parameters simultaneously in order to minimize the errors between the ab initio data and our model. The ab initio data for the determination of $h_{BrSiBr}$ were obtained from the calculations performed for the Br–
Si–Br cluster (S = 1) by varying \( \theta_{\text{BrSiBr}} \) and maintaining the bond lengths constant, where the potential energies for the optimized configuration of \( r_1 = r_2 = 2.2833 \, \text{Å} \) and \( \theta_{\text{BrSiBr}} = 103.16^\circ \) were set to be zero as the common reference values for the \textit{ab initio} data and our model. The potential curves with the optimized parameters and the \textit{ab initio} data are shown in Fig. 5. Similarly, the parameters for \( h_{\text{BrSiSi}} \) were also determined on the basis of the \textit{ab initio} data obtained by scanning \( \theta_{\text{BrSiSi}} \) for the Br–Si–Si cluster (S = 6). The \textit{ab initio} data and our model for this case are summarized in Fig. 6, where each zero reference for the \textit{ab initio} data and our potential model is the potential energy of the optimized configuration of \( r_1 = 2.2790, \ r_2 = 2.3817 \, \text{Å}, \ \text{and} \ \theta_{\text{BrSiSi}} = 117.64^\circ \). For \( h_{\text{SiSiSi}} \), we used the parameters modified by Watanabe \textit{et al.},\textsuperscript{1,6} which are slightly different from the original SW parameters. All the parameters obtained in this study are summarized in Table I.

Potential energies for small stable clusters such as SiBr\(_x\) (x = 1–4) are calculated by using our model and compared with the \textit{ab initio} data by using GAUSSIAN03, as shown in Table III. Since our model does not include the dependency of the two-body functions on the surrounding bond number (i.e., for more than three multibody interactions), the bond energies and bond lengths are almost identical for all the cases. The bond energies in SiBr\(_4\) clusters are approximately 15% higher than those obtained from the \textit{ab initio} calculations.

In this study, we determined the parameters on the basis of potential energy data for isolated small clusters. However, the etching characteristics, particularly the spontaneous etching of Si by low-energy room temperature particles, should be determined by highly precise potential barriers for ion penetration or absorption on the surface Si atoms. In fact, previous studies have clarified that for more realistic simulation results, and the SW models must be substantially improved.\textsuperscript{4,5} Similar discussions for our model for Si/Br systems will be part of our future studies.

IV. TEST SIMULATIONS

Sample MD simulations of Si etching by high-energy Br\(^+\) bombardment were performed by using our potential
The initial target temperature is 300 K, and the atoms in the bottom layer are rigidly fixed in order to prevent entire simulation cell from drifting.

High-energy atoms are injected from randomly selected horizontal locations immediately above the target in the direction normal to the surface. (Since high-energy ions impinging on the surface are expected to be neutralized near the target surface due to Auger emission, we only consider the charge-neutral atoms as the injected species, i.e., these ions refer to neutral atoms with high translational energy.) Here, the impinging atom is either $\text{Br}^+$ or $\text{Cl}^+$ with a translational energy of 10–150 eV. It is sometimes more convenient to measure the dose of impinging particles in monolayer units, with 1 ML corresponding to 72 impinging particles. After the injection of each atom, we allow the system evolve for 0.7 ps to reduce the temperature of the target to the initial temperature (i.e., 300 K). The target is repeatedly bombarded by a single high-energy particle for approximately 1800 times (approximately 25 ML). Statistically averaged data such as atomic distribution as a function of depth, etching yields, and stoichiometry were obtained by averaging over 15 ML impacts after 10 ML irradiations.

The typical surfaces (after the 10 ML impact) during Si etching by $\text{Br}^+$ and $\text{Cl}^+$ ions with a translational energy of 150 eV are shown in Figs. 7(a) and 7(b), respectively, where the white, blue, and green spheres correspond to Si, Br, and Cl, respectively. Similar to the previous studies, Feil’s potential model was adopted for the MD simulation of Si etching by $\text{Cl}^+$. The atomic distributions are also shown in Figs.

![Diagram](image_url)

**FIG. 6.** (Color online) Potential energies for the Br–Si–Si configuration obtained from GAUSSIAN03 (diamonds) and our potential model (solid line).

**FIG. 7.** (Color online) Typical surface structures during etching using 150 eV monoenergetic (a) Br$^+$ and (b) Cl$^+$ beams. White, blue, and green spheres indicate Si, Br, and Cl, respectively.

**TABLE III.** Si–Br bond energy, Si–Br bond length, and angle spanned by two Si–Br bonds obtained from GAUSSIAN03 and our potential model. $S$ indicates the spin multiplicity used in the calculation by GAUSSIAN03.

<table>
<thead>
<tr>
<th>Bond</th>
<th>Bond energy (eV)</th>
<th>Bond length (Å)</th>
<th>Bond angle (deg)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Gaussian Model</td>
<td>Gaussian Model</td>
<td>Gaussian Model</td>
</tr>
<tr>
<td>SiBr(S=2)</td>
<td>3.68 3.67</td>
<td>2.27 2.32</td>
<td>... ...</td>
</tr>
<tr>
<td>SiBr$_2$(S=1)</td>
<td>3.62 3.67</td>
<td>2.28 2.32</td>
<td>103 105</td>
</tr>
<tr>
<td>SiBr$_3$(S=2)</td>
<td>3.09 3.67</td>
<td>2.25 2.32</td>
<td>110 105</td>
</tr>
<tr>
<td>SiBr$_4$(S=1)</td>
<td>3.17 3.66</td>
<td>2.22 2.32</td>
<td>109.5 109.5</td>
</tr>
</tbody>
</table>
Cl atoms can penetrate the Si substrate to a depth of more than 40 Å, as shown in previous studies. In contrast, Br atoms cannot penetrate the Si lattice and, hence, remain at the vicinity of the surface that leads to relatively flat surface for Br beams compared with Cl beams. As a result, the total halogen coverage (total halogen content in the simulation cell) for the Br impact is smaller than that for the Cl impact. This tendency qualitatively agrees with the results of the experiments performed by Cheng et al. using Cl$_2$/HBr plasmas. Such a difference in the etching characteristics may be essentially caused by the difference in the chemical properties, i.e., potential functions. The details will be published elsewhere.

The Si etching yield and stoichiometry of the etching products SiBr$_x$ and SiCl$_x$ ($x = 0$–4) are summarized as a function of the beam energies in Fig. 9. Si yields (per ion impact) were estimated from the total amount of Si atoms sputtered as etching products: Si$_x$Br$_y$ and Si$_x$Cl$_y$ ($x \geq 1$, $y \geq 0$). During beam etching, the halogen flux into the simulation cell equals the total halogen content in the etching products, i.e., both these values are equal to 1 (per impact) after the etching characteristics are statistically stabilized. The estimated Si yield for the Br$^+$ bombardment is smaller than that for the Cl$^+$ beam afforded a large amount of Si and SiCl products. It is considered that Si is sputtered more physically because of the roughness of the surface (i.e., microscopically off-angle beam injection to surface atoms). Further discussions, particularly, the relation between potential barriers for ion penetration and the simulation results, have been reported by Iwakawa et al.

V. SUMMARY

In summary, we have developed a potential model for Si–Br systems to perform classical MD simulations. Our potential model is based on the well-known SW model, while the parameters are determined from the data for small clusters containing up to three atoms. This model enables us to simulate Si etching by Br$^+$-containing plasmas. The preliminary simulation results of Si etching by monoenergetic Br$^+$ beams qualitatively agreed with the experimental results. This simple systematic procedure for constructing parameters can be easily applied to other unexplored systems.
ACKNOWLEDGMENTS

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