Molecular dynamics simulations of 30 and 2 keV Ga in Si

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Focused Ga^+ ion beams are routinely used at high incident angles for specimen preparation. Molecular dynamics simulations of 2 and 30 keV Ga bombardment of Si(011) at a grazing angle of 88° were conducted to assess sputtering characteristics and damage depth. The bombardment of atomically flat surfaces and surfaces with vacancies shows little energy transfer yielding ion reflection. The bombardment of surfaces with adatoms allows for the coupling of the energy of motion parallel to the surface into the substrate resulting in sputtering. The adatom and one other Si atom eject, and motion in the substrate occurs down to a depth of 13 Å. Experimental evidence shows that sputtering is a reality, suggesting that an atomically flat surface is never achieved. [DOI: 10.1116/1.2756541]

I. INTRODUCTION

Focused ion beam (FIB) specimen preparation methods continue to dominate semiconductor and other materials systems where site specific sectioning is necessary. It is well known that depending on the ion incident angle, conventional 30 keV Ga^+ ions will impart tens of nanometers of surface damage into a target.[1] For a given target, the type and depth of ion damage depend on the ion species, the incidence angle, and the ion energy. In most experiments, the induced damage is accepted as an inevitable side effect to the FIB milling. For FIB milling, however, it is possible to reduce the damage by about a factor of 2 or more by using high incident angles (i.e., 88°) to the surface of interest compared to milling at normal incidence (i.e., at 0°) to the surface of interest. Indeed, most FIB sample preparation processes are performed at high incident angles to the surface of interest. To reduce further ion damage by a factor of 10 or more, the ion energy is reduced. For example, subangstrom information has been achieved in a FIB prepared Si specimen for high resolution transmission electron microscopy, where ~20 nm of 30 keV Ga^+ surface amorphization damage has been reduced to <2 nm of damage by polishing with 2 keV Ga^+.[2] In addition, the use of low energy 2 keV Ga^+ ions has also been shown to reduce ion mixing and implantation artefacts in samples prepared for atom probe analysis.[3]

Since FIB milling is becoming increasingly important for a plethora of applications, a fundamental understanding of ion-solid interactions at grazing angles is necessary. The traditional approach for estimating sputtering properties of high energy ion beams has been to use SRIM simulations.[4] Grazing angles, however, have very small collision energies in the direction perpendicular to the surface and it is well known that the binary collision approximation which is the heart of the SRIM simulations is not appropriate at low energies. Consequently we turn to molecular dynamics (MD) simulations of Ga on Si in an attempt to understand how surface characteristics influence sputtering and the implications for specimen preparation. The Si surface to be examined is (011) as it is the predominant surface used in sample preparation.

II. COMPUTATIONAL MODEL

The motion of Ga ion milling along the (011) surface of Si is modelled with (MD) computer simulations and schematically shown in Fig. 1.[5] Briefly, the classical equations of motion for all the particles in the system are integrated in time in order to follow the motions and velocities of each of the particles. The angle of incidence of the Ga ion is coplanar with (100) and 88° with respect to the [011] direction. The incident Ga has 30 or 2 keV of incident energy. 100 impact points on the surface were randomly chosen. The geometry of the model is illustrated in Fig. 1.

Choosing a sample size for these grazing incidence impacts is nontrivial as there is a long approach path before the atom actually strikes the surface. Initial test simulations indicated that very little energy is transferred to the substrate, thus a sample size of 49 Å × 54 Å or 252 atoms in the surface by 20 layers deep is sufficient to contain all the atomic motions. Periodic boundary conditions are applied in the lateral dimensions because, in fact, not much energy gets transferred to the substrate. The periodic boundary conditions keep the edges of the sample from reconstructing during the course of the simulation. The bottom layer of the sample is held rigid. The initial positions of the atoms are at their bulk terminated equilibrium positions and their initial velocities are zero.

The choice of the interaction potentials for the Ga and Si particles is motivated by the conventional wisdom that the Ziegler-Biersack-Lindhard (ZBL) repulsive interaction[4] is appropriate for the hard collision portion of the dynamics. For the Si–Si chemical bonding interaction we chose to use the third Tersoff potential[6] as we have had prior experience

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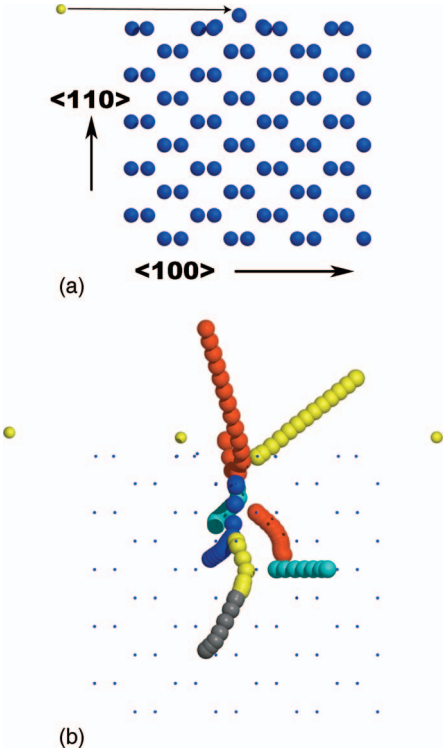

FIG. 1. Atomic arrangement of a (100) section through a (011) surface (a) with the adatom positioned 1.5 Å above the surface. The Ga particle is yellow and impinges from the left. Only a small portion of the atoms used in the simulation are shown. (b) shows a time sequence of atomic positions every 2 fs of all the atoms that moved more than 3 Å within the first 125 fs. The color assignment is arbitrary. See text for further discussion.

using this potential for sputtering simulations.[7] The repulsive wall of the Tersoff potential is connected to the ZBL potential by a cubic spline in the distance range of 0.30–0.95 Å. Simulations of the sputtering yield of 5 and 30 keV Ga normally incident on an amorphous target give values within a factor of 2 of the SRIM yields,[4] thus we feel comfortable that the potentials are reasonable.

In addition to the perfect (011) type surface, two surfaces were constructed in which one surface atom was removed from the surface and one in which one adatom was placed on the surface at a height of 1.5 Å above the surface and bonded to two surface atoms as shown in Fig. 1. These surfaces are designed to give a simple defect as possible in order to explore the effect on the scattering process.

III. RESULTS AND DISCUSSION

A. Scattering from a smooth (011) Si surface with no defects

For scattering of the Ga particle at 88° angle of incident from the surface normal, a total of 100 different impact points were calculated for 2 and 30 keV Ga energy. In all cases the Ga particle reflected from the surface and caused no sputtering of Si atoms. For 2 keV incident energy, the Ga particles each lost less than 2 eV of energy. For the 30 keV incident energy, the Ga particles lost between 28 and 35 eV of energy. Although there is sufficient energy imparted to the surface to eject an atom, the molecular dynamics simulations do not show that ejection actually occurs.

TABLE I. SRIM simulations of 1000 Ga^+ ions in Si at 88°.

	Sputter yield (at./ion)	Average sputtered atom energy (eV)	Percentage of backscattered ions
30 keV	25	206	64%
2 keV	5	77	65%

The magnitude of the energy transfer can be understood by considering the reflection of a Ga particle from a flat, smooth surface. In this case, the important amount of energy is the kinetic energy associated with the perpendicular velocity component. For 2 keV total incident energy, the perpendicular energy is only 2.4 eV. For 30 keV total incident energy, the perpendicular energy is 36.5 eV. The incident particle in the MD simulations is thus transferring an amount of energy corresponding to the perpendicular motion and is retaining the vast majority of the energy parallel to the surface. Although the surface roughness does alter the trajectory a bit, the change in parallel motion is negligible. Most importantly, the energy associated with the motion parallel to the surface cannot couple into the substrate. Since 100% of the incident ions were reflected or backscattered, no ions are implanted into the surface.

For comparison, Table I below shows results from Monte Carlo simulations using the stopping and range of ions in matter (SRIM) calculations of 30 and 2 keV Ga bombardment in Si at 88° angle of incidence.[4] The values obtained from SRIM simulations indicate a sputter yield of 25 at 30 keV and 5 at 2 keV. In addition, the percentage of backscattered ions is greater than 60% at both 30 and 2 keV. The SRIM calculated sputter yield values and percentage of backscattered ions values deviate significantly from the MD simulations presumably because an assumption of the SRIM calculation is that the target is amorphous and consequently the surface is not atomically smooth.

B. Scattering from a (011) Si surface with defects

To examine surface roughness, vacancy and adatom configurations were examined. The surface vacancy does not appear to influence the dynamics, and all incident Ga particles are reflected as is the case for the perfect surface. The adatom, however, does provide a mechanism whereby the energy associated with the motion parallel to the surface can couple into the substrate. As shown in Fig. 1(a), the adatom shown in the (100) planar section is initially 1.5 Å above the (011) surface. Figure 1(b) gives atomic positions every 2 fs for the atoms that moved more than 3 Å from its initial position. Each atom is assigned a specific color. The 30 keV Ga atom (small yellow sphere) hits the adatom (red sphere), transferring 275 eV of energy. The adatom reflects off the second layer striking a first layer atom (large yellow sphere)

on the way up and ejecting it. The adatom (red sphere) ejects with 76 eV of kinetic energy and the first layer atom (yellow sphere) that is sputtered has 20 eV of kinetic energy. The total motion in this trajectory includes a sequence of collisions involving motion into the eighth layer, corresponding to a distance of 13 Å.

These results show that some surface roughness is necessary for sputtering to occur at very grazing angles of incidence (i.e., high incident angles). Since we know from experiments that Si sputtering does indeed occur at 2 and 30 keV Ga energies,[2] we can infer that surface roughness is inevitable for ion polishing at high incident angles even at low energy. Therefore, it is unlikely that FIB polishing can create a nonfacetted or atomically smooth surface.

IV. CONCLUSIONS

Ultimately, to assess the effect of defects on the milling process, one would need to perform a series of MD simulations where a steady state interface is obtained. This simulation would be a monumental computational effort. What we have demonstrated, nonetheless, is that sputtering from an atomically flat surface is essentially impossible. However, adding even a single adatom allows for coupling of the Ga energy into the substrate and can eject atoms or mill the surface. The milling process is thus intimately intertwined with surface irregularities.

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