Gallium-Induced Milling of Silicon: A Computational Investigation of Focused Ion Beams

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Abstract: Molecular dynamics simulations are performed to model milling via a focused ion beam (FIB). The goal of this investigation is to examine the fundamental dynamics associated with the use of FIBs, as well as the phenomena that govern the early stages of trench formation during the milling process. Using a gallium beam to bombard a silicon surface, the extent of lateral damage (atomic displacement) caused by the beam at incident energies of both 2 and 30 keV is examined. These simulations indicate that the lateral damage is several times larger than the beam itself and that the mechanism responsible for the formation of a V-shaped trench is due to both the removal of surface material, and the lateral and horizontal migration of subsurface silicon atoms toward the vacuum/crater interface. The results presented here provide complementary information to experimental images of trenches created during milling with FIBs.

Key words: molecular dynamics, FIB, gallium, silicon

INTRODUCTION

Focused ion beams (FIB) have become an indispensable tool for many applications, including sample preparation and secondary electron imaging, as well as several types of "nanomachining" techniques (Giannuzzi & Stevie, 2005). One of the most extensive applications of these beams is their use in the research, development, and fabrication of semiconductors in the electronics industry (Prewitt & Mair, 1991; Orloff et al., 2003; Giannuzzi & Stevie, 2005). The range of tasks in this area includes circuit editing, mask and circuit repairs, and failure analysis.

As the complexity of modern electronics continues to increase rapidly, the techniques afforded by the FIB instruments are being driven to their physical limits. Circuitry is becoming so small that the intrinsic damage caused by these beams is on the same scale as the circuit features themselves. To keep up with these demands, an investigation into the fundamental dynamics that govern these experiments is needed.

We have chosen to use molecular dynamics (MD) simulations to investigate these systems. Molecular dynamics simulations have been used extensively to model the dynamics of energetic particle bombardment of solids (Urbassek, 1997; Garrison, 2001; Webb et al., 2001; Haddeman & Thijsse, 2003; Postawa et al., 2005; Krantzman et al., 2007;

Russo et al., 2007; Ryan et al., 2007). If one is interested in modeling the ejected atoms and molecules as measured in experiments, the simulation strategy is to have each incident particle bombard a pristine sample. Multiple simulations are performed, each having a slightly different aiming point of the incident particle on the substrate. The results of all the ejected particles are averaged for comparisons to experimental data. This strategy works well for modeling ejected particles because they tend to arise from near the surface due to the nature of the energy deposition (Delcorte & Garrison, 2000). Any energy deposited deep in the sample does not promote ejection; thus this motion does not need to be followed. Modeling milling of a material, however, requires that the same sample be repetitively bombarded and that the history of how one particle disrupted the sample influences the environment for the next bombardment event. The fact that more dynamics must be monitored means that system size needs to be larger and/or the incident energy must be kept small.

Several MD simulations have been performed that have effectively modeled repetitive bombardment events similar to the type of behavior present during FIB milling applications. Humbird and coworkers have carried out numerous simulations to examine the atomistic behavior of silicon etching via bombardment with fluorine, chlorine, and argon (Humbird & Graves, 2005; Humbird et al., 2007). Similar simulations were also performed by Feil et al. (1991) and Schoolcraft and Garrison (1991). Haddeman and Thijsse (2003) and Thijsse et al. (2004) have utilized high dose

computational techniques as well to explore the sputtering behavior of successive bombardments. These simulations have all been conducted using low energy impacts in the range of tens to hundreds of electron volts and small sample sizes on the order of a few hundred cubic angstroms with periodic boundary conditions. The imposition of periodic boundary conditions is appropriate for depth profiling or etching experiments where one is not particularly interested in the edges of the trench. In the current study, we have developed a protocol to follow the essential motion due to bombardments in the tens of kiloelectron volt range, as well as removed the need for periodic boundaries in order to study the formation of nanometer scale trench features.

The system we have chosen to study is crystalline silicon due to its prevalence in the semiconductor industry. Using a gallium beam, the objective is to model the removal of material in the near surface region, which leads to the formation of a trench as seen in experiments involving beams of this type, as well as to examine the dynamics that govern the narrowing of the sidewalls near the bottom of the trench (Ishitani et al., 1998, 2004; Lehrer et al., 2001; Rubanov & Munroe, 2004). Specifically, we use two identical Si(100) substrates that are repetitively bombarded with a circular beam of randomly oriented gallium atoms with either 2 or 30 keV of incident energy per atom. These energies were also chosen due to their prevalence in experiment/industry. A protocol for computationally managing the successive bombardment, removal of incident particles, and the relaxation/equilibration of the sample between hits has been developed for this study and will be explained in detail below.

The success of our investigation at producing the trenches found in experiment has shed light on the types of phenomena associated with their formation and the dynamics responsible for their shape. A comparison of the systems at these two incident energies as well as analysis of the extent of damage caused by these beams have been performed and will be discussed along with the remainder of the results.

COMPUTATIONAL DETAILS

Molecular dynamics simulations have been prevalent in a wide variety of applications involving the classical atomic motion of experimentally significant systems. The essence of the molecular dynamics procedure utilized here involves the numerical integration of Hamilton's equations of motion through time, which yields the positions and velocities of all the particles at each time step. A more detailed description of this MD scheme has been explained elsewhere (Garrison, 1992, 2001).

To simulate a high dose and high-energy bombardment event, there are several physical and technical issues that must be addressed, and thus several strategies have been developed to make these simulations both feasible and
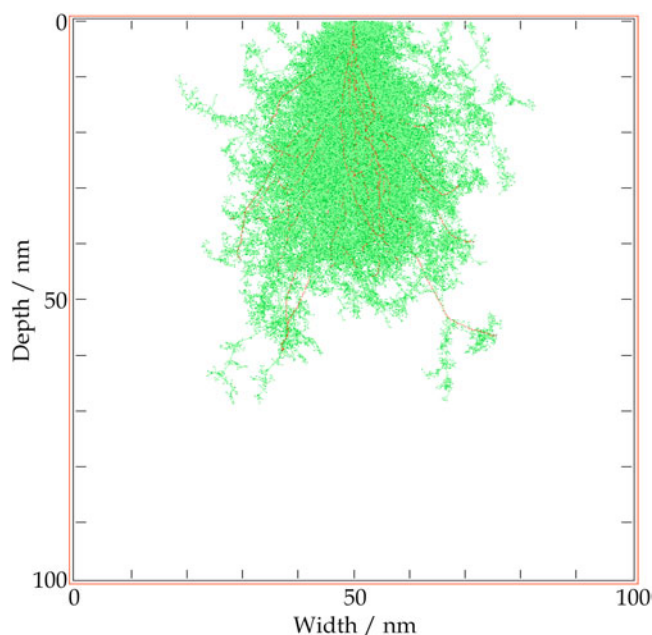

Figure 1. TRIM calculation of one hundred 30-keV gallium impacts on silicon.

physically relevant. Figure 1 shows the trajectories of one hundred 30-keV gallium impacts on a silicon sample as calculated using TRIM (Ziegler et al., 2008). All the incident ions strike at one point, that is, a point source beam. Using this information, a full MD simulation would require a sample roughly equal in volume to the field of view of Figure 1, or $(100 \text{ nm})^3$. Due to computational limitations, however, a sample of this size is not practical to simulate. Moreover, our objective is to examine the formation of the trench in the near surface region, thus all the motion deep in the sample is secondary to the process of interest. Therefore, we have implemented a scheme in which the gallium particles can be turned on or off with respect to their interaction potential with the rest of the sample, allowing us to use tractable sample sizes that emphasize the region of the sample in which we are interested.

Initially, each gallium particle in the beam is placed in a reservoir above the surface and made to be invisible to the rest of the sample, having no velocity and no interaction with other particles. Each gallium particle is individually turned on, having its interaction potentials activated and velocity changed to match a kinetic energy of either 2 or 30 keV depending on the study. As the gallium particle approaches the bottom of the sample (2.5 nm above the bottom), it is then turned off again. This prevents both the deformation of the sample and the reflection of the gallium particles, while still allowing for a physically relevant investigation of the surface and near surface region dynamics up to a depth of 7.5 nm.

Using this reservoir technique and applying the automation of successive bombardments requires that there be a
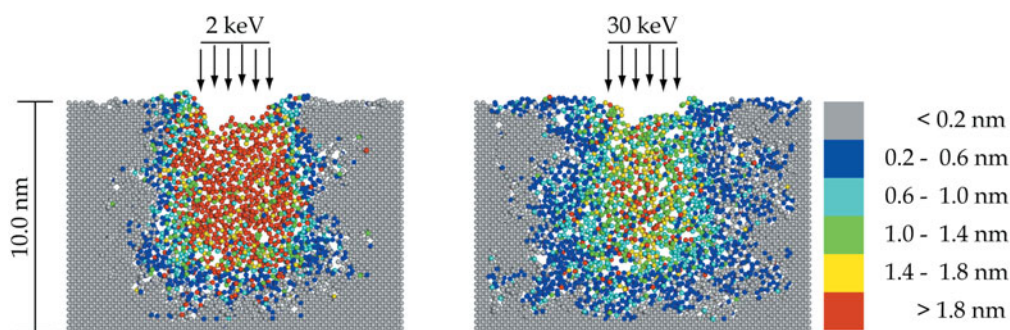
Figure 2. 20-nm cross sections of the two Si(100) samples after 425 impacts. Si atoms are colored by the distance displaced from their initial position.

sufficient amount of time between impacts to accurately represent an experimental beam. This condition is problematic, however, because the experimental timescale between impacts is orders of magnitude larger than the picosecond scale of the simulations. To solve this issue we have implemented a scheme similar in spirit to that of Haddeman and Thijsse (2003). Before each impact event can be started, the simulation must wait until the stochastic layer has sufficiently dampened the sample's temperature back to its original value of 300 K. Once this relaxation has occurred, the next gallium particle is activated from the beam.

The projectile beam is comprised of gallium particles randomly arranged within a 3-nm-diameter circular area, 2.5 nm directly above the center of the sample. This beam size has been chosen based on the approximately 5-nm-diameter beams used in experiment, coupled with the need to keep the sample size as computationally feasible as possible. The surfaces are then bombarded successively with either a 2- or 30-keV gallium projectile one at a time. For the samples, two identical cylinders, each composed of ~83,000 silicon atoms arranged in a (100) diamond lattice measuring 10.0 nm deep and having a radius of 7.23 nm, are used for this study. These dimensions were chosen to make the sample as large as possible while still maintaining a tractable computation time and also allowing us to study the early stages of a trench with dimensions on the order of the beam itself. Rigid and stochastic regions measuring 0.5 and 2.5 nm, respectively, are employed around the outer edge and bottom of the samples to maintain its shape, simulate the energy dissipation into a larger bulk, equilibrate the sample between impacts, and prevent the artificial reflection of pressure waves back toward the center. The intermolecular forces used to describe these systems are comprised of empirical potentials. Because our primary concern for this investigation is the development of a trench and not the chemistry associated with the incident beam, both the Si-Ga and Ga-Ga interactions use a purely repulsive Ziegler-Biersack-Lindhard (ZBL) potential (Ziegler et al., 2008). For the Si-Si interaction we have chosen a potential that has been shown in the past to reproduce the chemistry

of silicon reasonably well; a Tersoff-3 potential that was splined to a ZBL potential at 0.358 and 0.5430 Å was used (Tersoff, 1989).

Results

A cross-sectional view of both the 2- and 30-keV samples is shown in Figure 2 for a total of 425 Ga impact events. Each image is colored to represent the net displacement of silicon atoms from their original lattice position. From these images, several key characteristics of the bombardment event are illustrated, as well as several qualitative differences in the dynamics due to the two energies. First, in both cases a trench in the sample is clearly present. The trenches have the characteristic V-shape of many of the experimental profiles (Ishitani et al., 1998, 2004; Lehrer et al., 2001; Rubanov & Munroe, 2004; Giannuzzi & Stevie, 2005). Second, there is considerable disruption directly below where the beam impinges giving rise to material that has a lower density than crystalline silicon. Third, there is a slight mounding of material along the rim of the trench, an observation also seen in experiment (Ishitani et al., 1998, 2004; Lehrer et al., 2001; Rubanov & Munroe, 2004; Giannuzzi & Stevie, 2005). For the 2-keV bombardment, we find that almost all the energy is deposited within the active region of the sample (above 7.5 nm) and the method of turning off the gallium particle when it is within 2.5 nm of the bottom is rarely implemented. Consequently, there is considerable motion and disruption within the area directly below the beam as shown by the predominant red color of particles indicating that they have moved more than 1.8 nm. Conversely for the 30-keV bombardment, virtually all the incident gallium particles are removed from the bottom of the sample still possessing ~29 keV of energy, thus they only deposit ~1 keV in the target. This lower amount of energy deposited directly below the beam is consistent with the observation that individual atoms are not displaced as far from their original positions as in the case of the 2-keV simulation. The 30-keV beam has
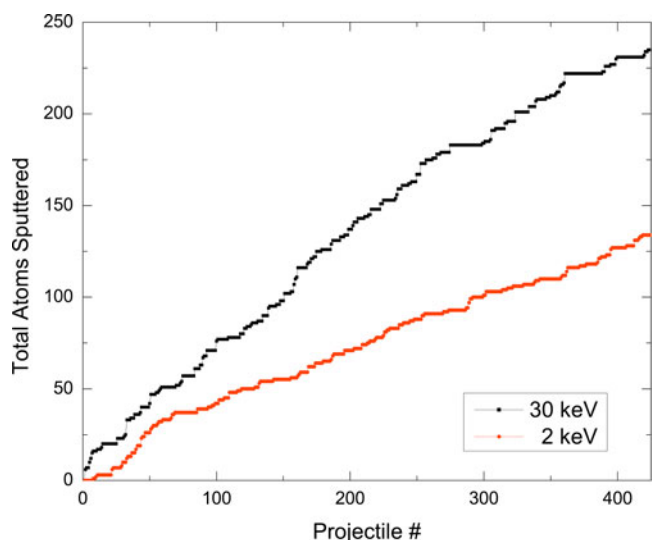
Figure 3. Total sputter yield for 2- and 30-keV gallium on silicon as a function of Ga impacts.

a larger extent of lateral damage throughout the silicon than the 2-keV beam as is consistent with TRIM calculation for these two energies (Giannuzzi & Stevie, 2005). There are different length scales considered in these two figures. Figure 1 (TRIM) depicts a view of 100 nm per side whereas Figure 2 (MD) is zoomed into a dimension of 10 nm deep and 15 nm in diameter. The MD simulations clearly show different damage and mixing characteristics in the region directly below where the beam impacts. The two approaches thus complement each other with the MD giving a close-up view near the impact region and the TRIM calculations giving the long-range perspective of the motion.

The two trenches shown in Figure 2 appear to be approximately the same size with perhaps the 2-keV trench being slightly larger. By examining the total sputtering yield for the two systems (Fig. 3), the 30-keV beam has removed two times the amount of silicon as the 2-keV beam for the 425 impact condition shown in Figure 2. To understand this information, we have examined the original positions of the sputtered material. Figure 4 illustrates a top-down and side view of the original lattice positions of the ejected atoms for both the 2- and 30-keV simulations. Although the higher energy system has removed twice the number of silicon atoms, the sputtered material has originated from a much larger and shallower volume across the top of the entire surface. Conversely, the lower energy beam has removed atoms with much higher precision from directly below the beam. The simulations thus suggest that a lower energy gallium beam would be more effective for creating a trench with minimal damage to the substrate. This conclusion, of course, ignores experimental details such as ability to focus the beam as a function of energy.

It is acknowledged that the yields calculated by the MD simulations are lower than those found in experiment for gallium bombardment of silicon. Experiments that have been performed using 15- and 25-keV gallium bombardment of an Si(100) sample determined a yield of 1.6 and 1.8 atoms per ion, respectively (Pellerin et al., 1990). The current simulations, however, produce a yield of approximately 0.6 atoms/ion. This difference is undoubtedly due to the empirical parameters of the interaction potential being optimized for systems near equilibrium and very high energies but not the intermediate regime where many important collisions take place. The potentials used, however, do describe a reasonable model system, and the conclusions drawn about the relative amount of damage for 2 keV versus 30 keV bombardment should be independent of the perfection of the potential for describing silicon.

The formation of a well-defined trench using the 30-keV Ga projectiles can be seen after 1,000 impacts in Figure 5. This trench is roughly 3 nm deep and can be seen along with the large amount of lateral damage throughout the sample. The trench formation with its tapered walls matches the characteristic shape of the trenches observed in the experiment (Ishitani et al., 1998, 2004; Lehrer et al., 2001; Rubanov & Munroe, 2004; Giannuzzi & Stevie, 2005) and has dimensions that are on the order of the beam size. An analysis of the source of this behavior is illustrated in Figure 6. These images depict the atoms that make up the 3 nm × 3 nm cylinder of the trench/vacuum interface for 30 keV as shown in Figure 5 at both the current time (1,000 impacts) and at their original positions. From this figure, it is apparent that the damage of the subsurface material has caused a significant amount of migration to occur within the sample. Due to this inherent projectile/sample interaction, there is migration of atoms laterally and vertically into the trench's interface with the vacuum. From the radial and horizontal color schemes of Figure 6, this migration can occur from a lateral distance of over 3 nm from the axis of impact and a depth of 6 nm from the surface. Migration and mixing of atoms in the substrate due to energetic particle bombardment is a well-known phenomenon. As the trench starts to develop, the corners are the natural place for the displaced atoms to aggregate. We expect this explanation to be valid independent of the projectile or substrate species. The mixing process as a cause for the trench shape means that every incident particle, regardless of impact point in the crater, has the opportunity to contribute to the infill. This is in contrast to the previously proposed mechanism of redeposition of atoms (Giannuzzi & Stevie, 2005) in which an incident ion must impinge on the minimal cross section of a sidewall, causing sputtering of material into and across the trench. For this process the incident particle must hit the sidewall, whereas statistically most incident particles are in the center of the beam and will miss the sidewalls.

Conclusions

Both 2- and 30-keV gallium incident beams are capable of producing a trench feature in silicon. The dynamics of how these two different energies remove material, however,
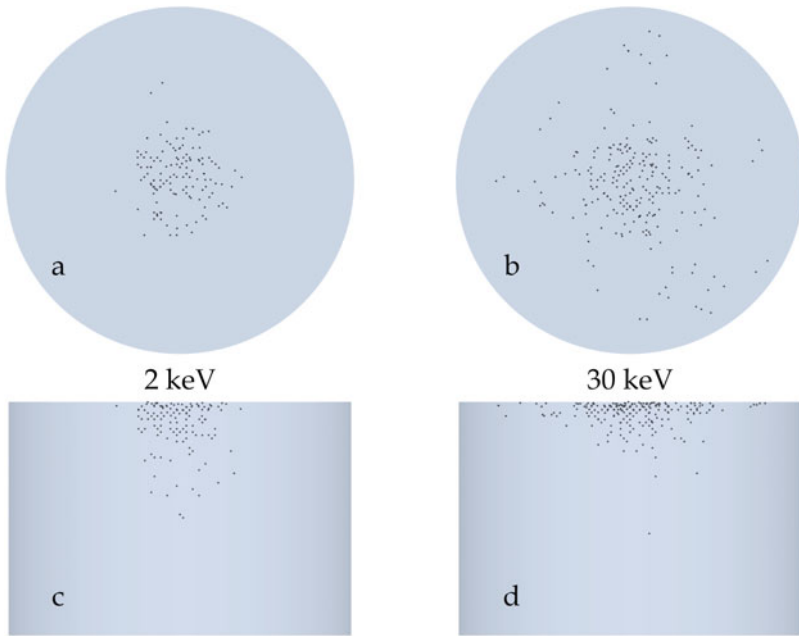
Figure 4. Top-down (**a, b**) and side views (**c, d**) of the sputtered material's original lattice position for both 2 and 30 keV, respectively. These images correspond to the cross sections of Figure 2 in that the sputtered material is after 425 impacts.
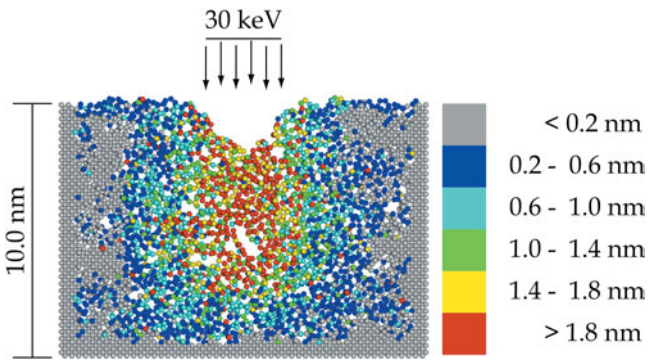
Figure 5. Cross-sectional view of the 30-keV sample after 1,000 impacts. Si atoms are colored using the same distance scale as in Figure 2.
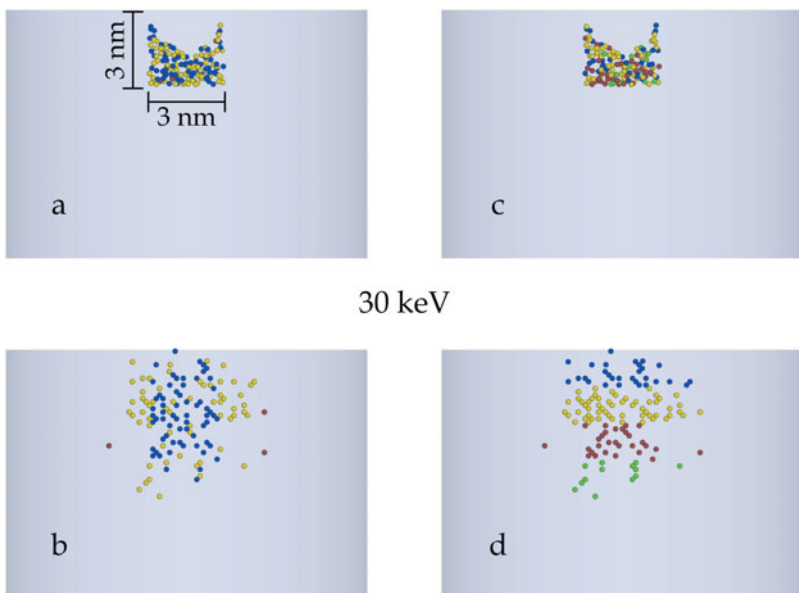
Figure 6. The volume of silicon atoms constituting the trench region after 1,000 impacts of 30-keV gallium and the same atoms shown at their original lattice positions at time zero. Coloring based on original locations. (**a, b**) Colored by 1.5-nm concentric rings, (**c, d**) colored by 1.5-nm layers.

varies significantly. Although 30-keV gallium has 15 times more energy per particle and removes twice the amount of material of the 2-keV system, much of its energy is deposited well below the near surface region. This behavior causes increased lateral and vertical damage as well as delocalized ejection from across the entire surface of the sample. The results of these simulations indicate that the lower energy beam is capable of creating a more well-defined trench, with reduced damage and more precise removal of material directly below the beam. In addition, our results indicate that migration of sample material both laterally and vertically due to the intrinsic damage created by the projectile/sample interaction contributes to the tapered sides and bottom of the trench interface region.

The MD simulations presented here provide insight into the physical processes that take place during FIB milling experiments. Using the techniques developed we have been able to successively bombard a sample and examine the dynamics of the system under various levels of accumulated damage, making high dose simulations at computationally feasible sizes and runtimes possible. With these tools, it should be possible to study many different types of multiple impact events that were previously impractical to perform.

Acknowledgments

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