keV PARTICLE BOMBARDMENT OF Si: A MOLECULAR DYNAMICS SIMULATION

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Molecular dynamics (MD) computer simulations of atomic ejection processes have been successfully used to predict a number of physical observables of direct interest to the SIMS community. For example, the energy and angular distributions of particles that eject from single crystal surfaces under keV particle bombardment can be accurately determined[1-3]. Because the simulations amass statistics from a number of unique trajectories they can also give information which is not readily obtainable experimentally such as the distribution of atoms ejected per impacting ion and the depth of origin of the ejected particles. They can also explain the mechanisms by which atoms are ejected.

Most MD simulations have been carried out for metal targets. This is because until recently it was only for close packed systems that realistic potentials were available. Semiconductors such as Si, GaAs or Ge have crystal structures which result in a tetrahedral arrangement of atoms and realistic potentials for these materials suitable for inclusion in a simulation code are now available. The existence of these potentials has enabled molecular dynamics simulations of Si to be carried out[4-6] and these have shown that the distribution of ejected atoms is dominated by the openness of the Si crystal rather than channelling and blocking by surface atoms as is the case for metals. Many SIMS applications involve analysis of semiconductors and here we discuss MD simulations of Ar^+ bombardment of Si, with particular emphasis on quantities of most interest in SIMS. The crystal faces chosen for study are the Si{110}, {100} and dimer reconstructed {100}(2×1) faces although we will concentrate on presenting results for the {110} face. Bombardment at both normal and oblique incidence will be considered; the differences in the ejection processes will be compared and the implications of these differences in interpreting SIMS data will be discussed.

THE MODEL

The simulations described here are based on a classical dynamics prescription where the interaction forces between the bombarding Ar particle and the Si atoms are derived from pairwise additive potentials and the interaction forces between the Si atoms are derived from many-body potentials. A full description of these potentials is given elsewhere[5,6]. The program is optimised for speed by using a fast numerical integrator of the classical equations of motion[7] and by implement-

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ing a moving atom approximation[5,8] which only includes particles in the calculation which have been hit sufficiently hard by another moving particle. These two aspects considerably increase the speed at which calculations can be carried out, which can be up to a factor of six compared to a full molecular dynamics simulation based on our previous integration algorithm for a target containing 500-2000 atoms.

The crystal size for the simulations presented here are 210 atoms in 7 layers for the bombardment of the Si{110} face at normal incidence. In order to speed up the oblique incidence calculations, a smaller target of 126 atoms in 5 layers was chosen for the Si{110} face although there was some evidence to suggest that the statistics were being affected by the relatively small target size particularly for bombardment near grazing incidence. As a related study[6] had its primary purpose to determine the peaks in the ejection yield (Y) as the incident polar angle ϑ varied and these could be observed with a smaller target, we have accepted some loss of accuracy in order to generate sufficient data within a reasonable time. For the {100} face the target had 155 atoms in 11 layers and for the dimer reconstructed Si{100}(2×1) face 128 atoms in 10 layers.

NORMAL INCIDENCE BOMBARDMENT

In this section we examine the results of calculations carried out when the incoming particles are incident normally on the Si crystal. The calculated yields as a function of energy varied between 0.03 per incident particle at 100eV to 0.43 at 1keV for the Si{110} face. At 1keV the calculated yield for the dimer reconstructed Si{100}(2×1) face was 0.66. For the unreconstructed {100} face the yield was 1.08. The experimental (higher dose) data collated by Zalm[9] gives an average value of around 0.9. The yields are calculated by averaging over a number of trajectories aimed at an area representative of the crystal as a whole. In all cases there were many trajectories where the ion was channeled and emitted no particles. It is for trajectories such as these that the moving atom approximation can save considerable computing time since only a few particles are set in motion in the surface layers. The calculated yields are much less than for face centred cubic (fcc) metals due to the more open nature of the crystal structure. At 1keV there was no evidence of high yield events which can occur at bombardment energies typical of SIMS experiments for metals[10]. The more open crystal structure is also reflected in the depth of origin of the ejected material. Calculations for the Cu{100}[11] face, which has a similar layer spacing to Si{110} show that 90% of ejected material originates in the first layer and 9% from the second layer at 1keV. These percentages are only slightly changed for energies up to 20keV. In contrast only 75% of material is ejected from the top layer of Si{110} at 1 keV with 19% from layer 2 and 6% from layer 3. For the dimer reconstructed Si{100}(2×1) face, the layer spacing is less and the figures are 46%, 31% and 16% respectively. Although these depths are deeper than for metals they still show that most of the material ejected in a typical SIMS experiment would originate in the top three atomic layers. We find no evidence of high energy particles emitted from deeper within the material as would be predicted by transport theories[12].

The angle integrated energy distributions of ejected material are found to peak at a fairly high value, for the Si{110} face at

7eV, for the Si{100} at 5 eV and for the dimer reconstructed Si{100}(2×1) face at 8eV. These values are greater than the cohesive energy of Si which is 4.63eV[13]. For metals the peaks in the energy distributions are typically 0.5-0.8 of the cohesive energy. Transport theories of sputtering[14] would predict that the peak position would be of the order of the energy cost to remove an atom.

The ejection pattern (angular distribution of ejected particles) along with the Si faces under bombardment and the azimuthal angle definition are shown in figure 1. The patterns are produced by calculating where ejected material crosses the unit sphere and projecting that point onto a plane parallel to the crystal surface. The pattern for the {110} face is shown for only the hatched Si atoms (Si_h). This is because for semiconductors such as GaAs or SiC, the Ga or Si atoms correspond to the position of the Si_h atoms and we wished to compare the data with experimental results of Ga ejection from a GaAs crystal. The results were in reasonable agreement[15]. The full ejection pattern for the Si {110} face can be obtained by reflection in the horizontal diameter.

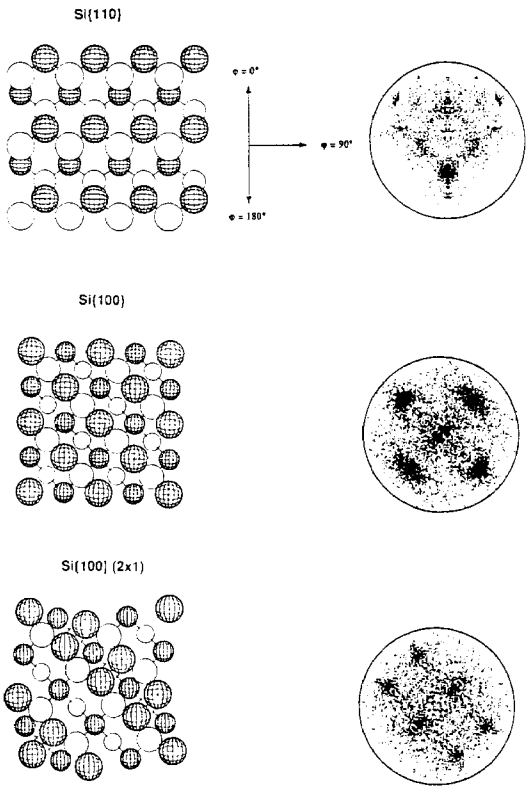

Figure 1. The crystal faces and ejection patterns (angular distributions) for normal incidence bombardment of Si. Only atoms ejected with energies up to 100eV are shown. The hatched circles (Si_h) would be the position of Ga atoms in a GaAs lattice. The larger circles represent the top layer atoms and the smaller circles the subsurface atoms which decrease in size with depth. The top figure for the {110} surface represents the angular distribution of only the (Si_h) atoms. The ejection patterns for the {100} faces are for all atoms.

Figure 1 shows that the main feature occurs at $\phi = 180^o$ (where ϕ is the azimuthal angle defined in figure 1) and at a polar angle of about $\vartheta = 40^o$ for the {110} face and is made up of atoms from all of the top three layers. A detailed discussion of the mechanisms which give rise

to the ejection pattern is given in reference [5]. Ejections can occur as a result of surface layer atoms hit from below by a second layer neighbor but also as a result of direct collisions with the ion or the first atom that the ion strikes. These mechanisms can be further illustrated by detailed examination of individual cascades. The patterns for the two {100} faces show preferential ejection along the $\phi = 45^o$ and 135^o azimuths, in agreement with the experimental observations of Macdonald[16]. Figure 2 shows a snapshot from one trajectory incident on the {110} face, after most of the atoms had been ejected. This trajectory is atypical since four atoms are ejected, about the maximum number observed at 1keV but is useful to examine mechanisms since atoms from all three layers are ejected. The figure shows that the second and third layer atoms are ejected close to the $\phi = 0^o$ and $\phi = 180^o$ azimuths whereas two adjacent first layer atoms are hit from below and ejected close to the bond direction. The ejection pattern shown in figure 1 consists of data obtained from 5400 unique trajectories such as this.

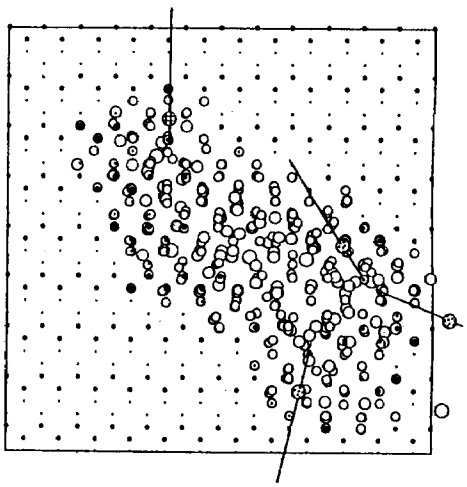

Figure 2. Snapshot of a normal incidence cascade for the {110} surface after 122 fs (1fs = 10^{-15}s). The cascade is viewed from above the surface layer. The small dots represent the unmoving atoms. The darker dots represent the first layer atoms. The moving particles are drawn as circles whose size increases according to energy for the three discrete ranges of < 10eV, < 100 eV and > 100eV. Three atoms have been ejected and are shown stippled. One atom is about to eject and is shown as hatched. The lines are drawn through the particles which are ejected back to their initial lattice positions. The two ejected atoms on the right of the diagram were originally first layer neighbors. The hatched atom at the top originates in the third layer and the stippled atom near the bottom of the diagram in the second layer.

OBLIQUE INCIDENCE BOMBARDMENT

In this section we stress some of the differences in the ejection statistics as the incidence angle ϑ varies. At normal incidence for 1keV bombardment no particle was found to be ejected with an energy > 100eV, 88% of ejected particles were emitted with energies less than 50 eV and 59% with energies less than 25eV. The incidence angle corresponding to the maximum yield, ϑ_{max} was calculated to be 72.5^o for $\phi =$

0^o. At this angle the calculated peak of the ejection energy is greater than at normal incidence. Statistics from 300 trajectories show that there is little variation in the distribution of low energy ejected atoms between about 4 and 20 eV. Analysis of the data shows that 56% of ejected particles are now emitted with energies > 25eV and 22% with energies > 100eV. They are also scattered preferentially in the forward direction. In a typical SIMS experiment, the particle detector will only have a small energy bandwidth and collection angle and it is important to bear in mind the contribution from the higher energy and forward recoils at oblique incidence. Measured yields may well not agree with those calculated for all energies and angles. However although the results show that a large number of high energy atoms are ejected, the increase in the yield at $\vartheta_{max} = 72.5^o$ compared to normal incidence is also made up from an increase in the number of low energy atoms. This suggests it would be better bombard at an angle ϑ_{max} in SIMS both for depth profiling and analysis.

A snapshot of the cascade from a typical trajectory is shown in figure 3. The lines represent the trajectories of the ejected particles and forward scattering is evident. Note that 8 atoms are ejected and up to 11 were found to be possible at this incidence angle. At normal incidence no trajectory emitted more than 5 atoms. Note also the formation of a dimer. The calculated yield at $\vartheta_{max} = 72.5^o$ is nearly 7 times the yield at normal incidence. At this incidence angle, energy is deposited much closer to the surface and non-linear cascade effects are important. This is illustrated for this cascade in the ejection of the dimer as a result of collisions between moving atoms. Analysis of the ejection mechanisms for this trajectory show that of the eight atoms ejected, three are as a result of direct hits with the ion, two are ejected by being hit by the first particle the ion strikes, one is hit from below by a second layer neighbor and the dimer is formed as a result of collisions between moving atoms. This trajectory illustrates the point that as the incidence angle increases from normal, the ejection mechanisms change. Neighbor/neighbor hits become less important and more material is ejected as a result of a direct hit with the ion or the first particle that the ion strikes.

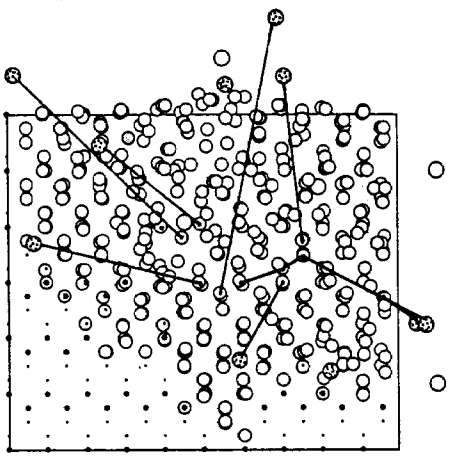

Figure 3. Snapshot of a 1keV cascade incident at ϑ_{max} and $\phi = 0$ after 203 fs for the {110} surface with the same particle size and pattern representations as in figure 2. The lines drawn on the diagram give the trajectories of the ejected particles. Note that one of the dimer atoms undergoes a series of collisions before ejection. The target size for this trajectory is slightly too small to contain the cascade laterally which spreads further than that shown in figure 2. at 1keV.

SUMMARY AND CONCLUSIONS

The simulations have enabled the underlying mechanisms for atomic ejection due to keV particle bombardment of Si to be determined at both normal and oblique incidence. The distributions are greatly influenced by the open nature of the tetrahedral crystal structure. The predictions of the simulations are shown to be in disagreement with those of transport theory both with regard to the depth of origin of the ejected atoms and their energy distribution. Ejection of both high and low energy recoils is increased at an incidence angle ϑ_{max} compared to normal incidence bombardment. Thus bombardment at ϑ_{max} should increase the analytical sensitivity in SIMS in addition to the depth profiling rate.

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