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Computer simulation of sputtering of gold targets using Sb and Sb_2 ions

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Abstract

It is well known that energetic impacts of Sb and Sb_2 ions on gold substrates give rise to high energy density collision cascades and potentially very high sputtering yields. A large component of the sputtering mechanism is due to the presence of a thermal spike which causes prolonged ejection of material with thermal energies. This phenomenon is investigated using molecular dynamics simulations. The energy dissipation mechanisms and the effects of molecular orientation are investigated. The overall sputtering yields are compared to experimental measurements. © 1999 Elsevier Science B.V. All rights reserved.

1. Introduction

There is a growing interest in the effects of molecular and cluster impacts on surfaces, particularly in the fields of implantation [1], sputtering [2], secondary ion mass spectrometry (SIMS) [3], deposition [4] and particle desorption mass spectrometry [5]. Single atom collisions with surfaces are normally quite well characterised using linear transport theory [6]. There are exceptions to this, for example when the deposited energy density of the impacting particle is so high that it causes all, or nearly all, of the target atoms to be set in motion then the ensuring collision spike can no longer be considered to be linear. This tends to happen for large mass ions impacting on dense targets. Antimony ions irradiating a gold substrate are typical non-linear cascade producers. Irradiation of surfaces by molecules and clusters, because a number of particles arrive at the same part of the target simultaneously, also produces non-linear cascade effects. It is well known, for example, that the sputtering yield increases non-linearly for many molecular impacts [7]. Recent [8] and previous work [9] has also shown that irradiation of Sb and Sb_2 ions on gold surface produces a non-linear scaling of the sputtering yield. We investigate here the difference between bombardment of a gold surface with monomer and dimer ions using molecular dynamics computer simulation.

2. Simulation method

The molecular dynamics simulation model used in this study has been described in detail in other

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publications [10,11] and so only a brief description will be given here. The simulation solves the equations of motion simultaneously for each particle and stores information on position, velocity and energy states at different time steps. The program uses the many-body potentials of Ackland et al. [12] to model the Au–Au interactions. The Sb–Sb and Sb–Au interactions are modeled by the Universal ZBL repulsive pairwise potential [13]. These interaction potentials do not describe the bonding nature of the Sb–Sb or the Sb–Au particles and so cannot be used to describe bonding configuration of the implanted Sb ions. Nor will they describe accurately the dissociation of the Sb_2 molecule. However, the energy of the interaction with the target surface is of such a magnitude that the dynamics are unlikely to be affected greatly by this lack of binding. Also these potentials are known to give a very good description of the high energy interactions and, so, should describe the initiation of the energy exchange with the surface atoms well enough to allow the formation of the ensuing collision cascade in the gold target. The gold target is then well described by the many body potential. Periodic boundary conditions are used at the lateral boundaries of the target cell, the surface and bottom layers are considered to be free. This allows sputtering of material and prevents unwanted reflection from the bottom layer of fast moving recoils. In general the target system is kept large enough to avoid the influence of the edges of the crystal. The target used in this study is a gold lattice of dimension 120 Å × 120 Å, consisting of 30 atomic layers. This contains approximately 25 000 atoms. The initial temperature of the lattice is 0 K. Impacts of Sb and Sb_2 on a single crystal (1 0 0) fcc gold surface are considered. We use a regular array of impact points in a symmetry zone of the crystal. We make average calculations over 164 trajectories for Sb and 328 trajectories for Sb_2. The number of trajectories is not high but by employing regular sampling rather than random trajectory sampling we reduce our errors [11]. In the case of the Sb_2 molecule we simulate impacts with the surface in two extremes: with the molecule aligned perpendicular to the surface; and with the molecule aligned parallel to the surface. Trajectories are chosen carefully in the latter case to avoid repeating impact conditions. The molecule is not considered to have any stored internal energy in the shape of rotational or vibrational energy prior to impacting the surface. This is unlikely to by high enough to cause major errors in the calculations as this internal energy will be low in comparison with the initial kinetic energy of the particle. The simulations have been performed at 50 keV for the Sb and 100 keV for the Sb_2 so that each particle will arrive at the target surface with the same velocity.

3. Results and discussion

Sputtering with molecules and clusters often leads to a non-linear enhancement of the sputtering yield. That is a dimer ion will often give greater than a factor of 2 increase in the sputtering yield. It is well known that high energy density deposition in the region of the surface of a target can result in non-linear sputtering yields and energy distributions of the sputtered particles which indicate they have a thermal origin. The Sb^+/Au system is known to exhibit this thermal spike behaviour even for impacts with a single ion.

In Fig. 1 we plot sputtering yield as a function of time for high yield, medium yield and low yield impacts for both Sb – Fig. 1(a) – and Sb_2 impacts – Fig. 1(b). There is little difference between the two. For the high yield sites the yield increases with time for a long time and is still rising even after 10 ps. The principle difference is that the high yield sites occur more frequently in the molecular impact case than the single atom case and some of the high yield are larger than in the non-molecular case. The enhancement in the yield comes from the fact that we double the number of high yield sites – on its own this would double the yield – and increase the "activity" of the high yield sites.

The sputtering yield for single atom Sb impact was found to be 41 atoms/ion and the yield for the Sb_2 to be 109 atoms/mol (or 54.5 atoms/Sb – 25% higher than would be expected from a linear relationship). For the very high yield simulations of the molecular impacts there is some evidence that we experienced a containment problem in which we created a hole right through the target region.

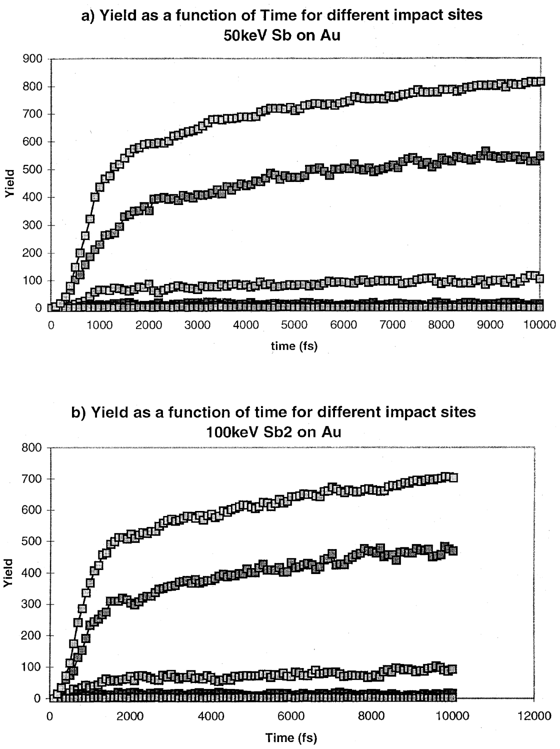

Fig. 1. Yield as a function of time for different impact sites for (a) 50 keV Sb on gold; (b) 100 keV Sb_2 on gold.

This will effect the degree of non-linearity seen between these results and we can expect the yields to be even higher from the molecular impacts.

In Fig. 2 we show the probability distribution of yields for Sb and Sb_2 impacts. We plot the

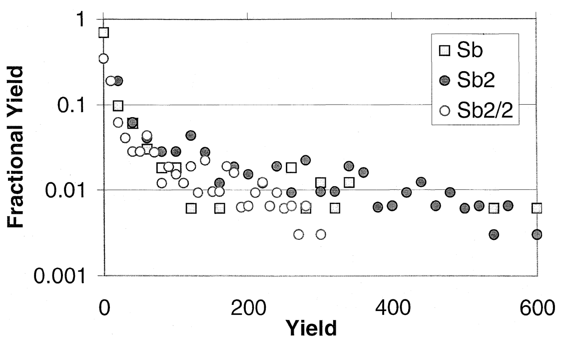

Fig. 2. Log of the sputtering yield probability function for a set of trajectories for 50 keV Sb and 100 keV Sb_2 on gold.

distribution on a log scale so we can see the small, but finite, probability of the high yield trajectories. There is very little difference between these distributions. The main thing to note is that the number of low yield sites is much reduced for the Sb_2 trajectories. The total number of high yield sites has more than doubled for Sb_2 and there are some sites which are higher than the highest single atom trajectories. The combination of these two effects gives rise to a higher than linear rise in the average sputter yield when going from Sb to Sb_2 impacts.

Fig. 3 shows sputtering as a function of impact point in the impact zone. It is noticeable that most of the yield comes from impacts close to the atoms of the surface and near surface. This is true also for impacts with the molecular ions no matter which way around the impacting ion is oriented, both vertically and horizontally aligned molecular impacts show only a broadening of the yield close to the target atoms. There are still a large number of impacts in the central region which produce little or no sputtering. The molecular ions as well as the atomic ions are channelling through the surface region and depositing their energy deeper in the target thereby not contributing to the sputtering yield.

In Fig. 4 we show the sputtering yield and the average "temperature" of the lattice as a function of time for a typical high yield event. The temperature of the lattice is taken from the mean square velocity of the particles in the target volume [14]. The figure shows that the temperature peaks as the sputtering yield slows its increase. Eventually the temperature reaches a steady value [15] and the yield continues to rise slowly for a prolonged length of time.

4. Summary and conclusions

Molecular Dynamics simulation of single atom and molecular antimony impacts on a gold target show that non-linear sputtering effects occur. In particular material is sputtered for long times after the impact and the yield per incident atom is greater for molecular species than single atom impacts. It was also found that the Sb/Au system gives rise to non-linear sputtering trajectories even

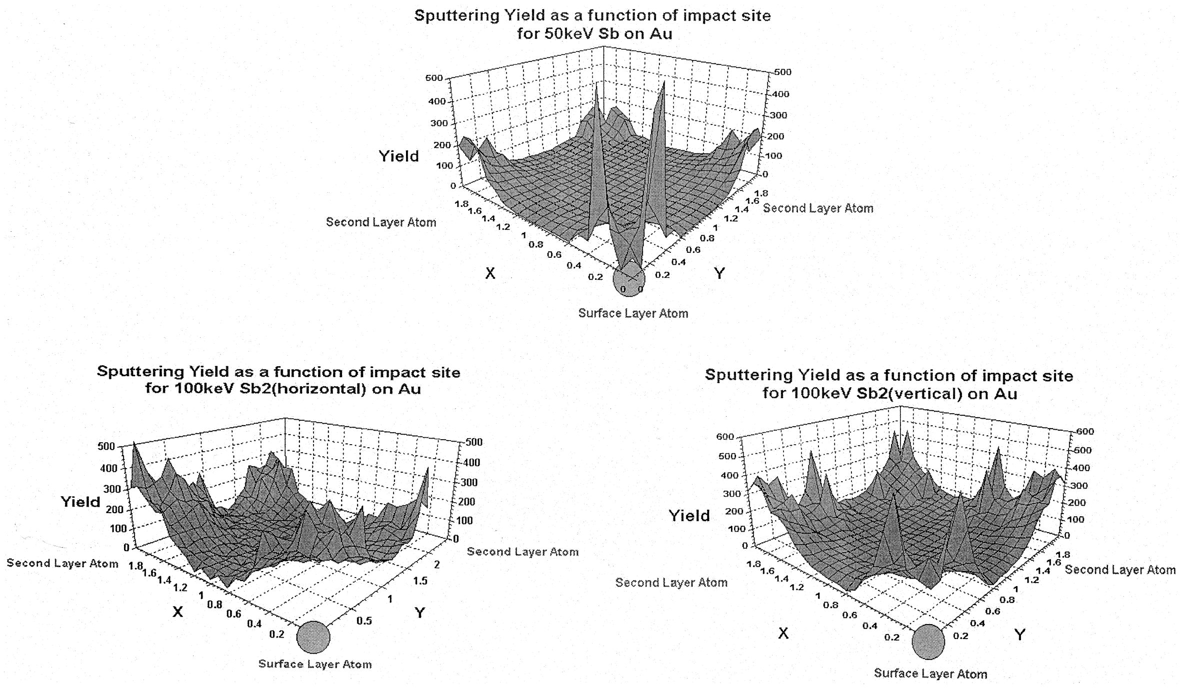

Fig. 3. Sputtering yield as a function of impact site for (a) 50 keV Sb on gold; (b) 100 keV Sb_2 – molecule horizontal – on gold; (c) 100 keV Sb_2 – molecule vertical – on gold.

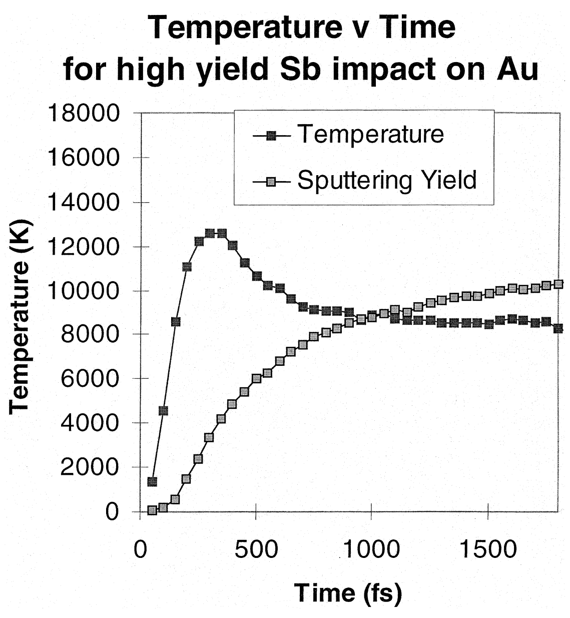

Fig. 4. Sputtering yield and target temperature as a function of time for a high yield impact site of a 50 keV Sb impact on gold.

for single atom impacts. The number of these increases when molecular ions are used. High yield sites give even greater yield number molecular impact. Both molecular and single atom ions show channelling effects.

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