Trapping and desorption of energetic Cu atoms on Cu(111) and (001) surfaces at grazing incidence

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Molecular-dynamics (MD) simulations of Cu atoms impacting both Cu(111) and (001) surfaces at grazing incidence have been performed to study trapping (or surface skipping), desorption, and energy dissipation. An energetic Cu atom ($10 \leqslant E \leqslant 100$ eV) can become trapped by the mean attractive potential above the surface, oscillating normal to the surface. While in this trapped state, it can traverse hundreds of Å as it dissipates energy to the surface. Until the atom either desorbs or comes to rest, it experiences an energy loss, that is piecewise linear in time, typically comprised of two or more linear regions. In each region, the energy loss rate, dE/dt, is approximately constant. The process can be characterized by two parameters: the desorption probability at each oscillation and an average energy loss rate (per oscillation) that is independent of energy. These parameter values are the same for both the (111) and (001) surfaces. A phenomenological model based on these parameters is presented, and the predictions of sticking probability, average energy transfer to the surface, and total distance traveled, agree with full MD simulations. The dependence of the desorption probability on the surface temperature was also studied. [S0163-1829(99)01339-9]

I. INTRODUCTION

The interaction of a gas atom with a surface is of fundamental importance to many areas of science and technology, e.g., catalysis, molecular sensing, etching, and thin-film deposition. As such, the study of the trapping and desorption of atoms and molecules on pristine metal surfaces has been a topic of interest for many years. The dependence of sticking probability on impact energy and angle of incidence has been shown to be important in modeling the growth of topographical features in the manufacture of semiconductor chips.[1] In these studies, summarized in Fig. 1, the sticking probability of Cu ions incident on a Cu(111) surface show an unexpected upturn as the impact angle approaches grazing incidence. We believe that this behavior is a consequence of a surface skipping phenomenon, and may be important for modeling the ionized physical vapor deposition (PVD) process used in the manufacture of integrated circuits.

Ohtsuki *et al.*[2] predicted the occurrence of skipping motion by an ion interacting with a smooth metal surface via an image charge potential. By computer simulation, they demonstrated that 30 keV H^+ ions could be trapped on a Ni(100) surface at grazing incidence ($\theta \leqslant 1°$ relative to the surface plane). Dodson[3] performed molecular-dynamics (MD) simulations of Si atoms ($10 \leqslant E \leqslant 100$ eV) impacting a Si(111) surface at grazing incidence and found that for angles of incidence below some critical value, the atom became trapped, or in his terminology, exhibited ''surface channeling.'' The critical angle for trapping depended on the ion energy; at 100 eV it was $\sim 7°$ with respect to the surface plane. He also found that the rate at which the ion dissipated kinetic energy to the surface was linear in kinetic energy, $dE/dx = -0.0193 + 0.000154E$, where the units are Å and eV. Snowdon *et al.*[4] claimed the first experimental observation of skipping motion. Using a beam of Si^+ ions with energies between 200 and 2000 eV, and impact angles between 1° and 14° with respect to the surface plane on Cu(111), several very weak, broad peaks (>100 eV full width at half maximum) in the energy distribution of the reflected beam were observed. These peaks, which were attributed to multiple skips on the surface, corresponded to energy losses of between 50 and 100 eV per impact. They concluded from their data that the kinetic energy dissipation rate to the surface, dE/dx, was proportional to the energy.

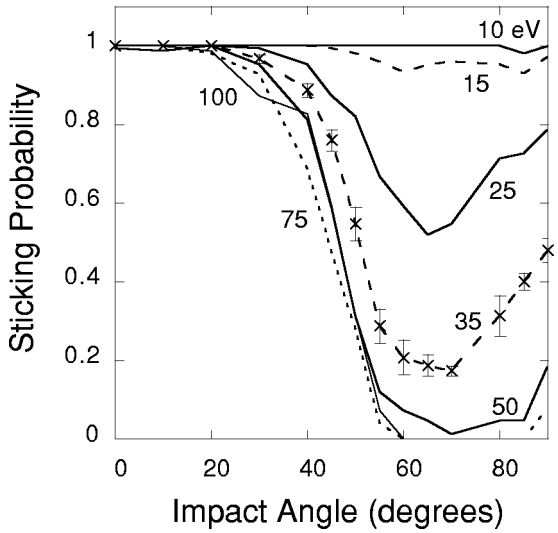

FIG. 1. Sticking probability versus angle of incidence (with respect to surface normal), parametric on energy (eV), for a Cu atom impacting a 300-K Cu(111) surface. Representative error bars, shown only for 35 eV, are one standard deviation of the mean.

Pfandzelter and Stolzle[5] reported experimental observation of the skipping motion of H^+ in the energy range of a few keV on the (0001) surface of graphite at angles of grazing incidence between 0.2 and 1.5 degrees. They observed distinct peaks in the reflected energy distribution that occurred at multiples of 1.5 to 5 keV depending on the incident ion energy. Winter and Sommer[6] obtained qualitatively similar reflected energy distributions from experiments of 50 keV H^+ on Al(111), at angles of grazing incidence, $\theta = 0.2°$, $0.4°$, and $0.5°$. They noted that for the smallest angle, $\theta = 0.2°$, distinct energy loss peaks occurred, but when the angle was increased to $0.4°$, these peaks disappeared. At a slightly larger angle, $0.5°$, broader energy loss peaks appeared at different positions. They interpreted this difference as the manifestation of two different scattering mechanisms. At the lowest angle, surface skipping was occurring, but at the largest angle, $0.5°$, subsurface scattering was operative. They attributed the results of Snowdon *et al.*,[4] which were obtained at angles of incidence between $1°$ and $4°$, to subsurface scattering rather than surface skipping.

Smith *et al.*[7] performed MD simulations for a Si^+/Cu(111) system for conditions similar to the experiments of Snowdon *et al.*[4] For 1000 eV Si^+ incident at $4°$ on Cu(111) at $T = 0$ K, they predicted only a single, narrow peak at 998 eV in the reflected energy distribution. When the crystal was disordered to simulate thermal vibrations at $T = 300$ K, the peak broadened on the low-energy side by ~ 10 eV. They found that only 5% of the incident ions remained trapped after the initial impact. Based on their estimate of the energy loss per collision of ~ 6.5 eV, the 1 keV ions experienced between 1 and 3 skips before desorbing. DiRubio *et al.*[8] observed multiple peak reflected energy loss distributions similar to those mentioned above, in experiments with Na^+ ions ($E = 100$ to 400 eV) incident on a Cu(111) surface at a much larger impact angle, $45°$. Their reflected energy distributions differed from previous work in that the height of the peaks increased with increasing energy loss. They attributed the peak with the greatest energy loss to ''quasisingle'' collisions with the surface and the lower loss peaks to multiple scatterings.

Considerable work has been carried out for atoms and molecules, at or near thermal energies, interacting with pristine metal surfaces via Van der Waals' forces.[9] Because of the very low-impact energies, comparable to the thermal energy of the surface, this work is not germane to the present work.

Here we report detailed results of MD simulations for Cu^+ ions incident on a Cu(111) $T = 300$ K surface at grazing incidence, and propose a simple phenomenological model, based on MD calculations, that describes the sticking probability and reflected energy distribution as a function of incident energy. We find that for grazing incidence impacts, an energetic Cu atom ($10 \leqslant E \leqslant 100$ eV) can become trapped by the mean attractive potential that exists above the Cu(111) surface. In this trapped state, the atom oscillates perpendicular to the surface with a period of ~ 0.2 ps. As the atom oscillates, it moves across the surface, dissipating its translational kinetic energy to the surface at a nearly constant average rate. It is the fast parallel motion that prevents the atom from forming a bond.

This phenomenon may be important for modeling the deposition and transport of material during ionized physical vapor deposition (PVD), a process widely used in the manufacture of integrated circuits. Typically, Cu is deposited by ionized PVD on features that have sidewalls nearly parallel to the incident ion beam. In previous work,[1] we presented sticking probabilities for Cu impacting a Cu(111) at angles up to $80°$, which showed an unexpected upturn between $60°$ and $80°$ with respect to the surface normal. (All angles specified hereafter are with respect to the surface normal.) Figure 1 shows an example of this behavior for Cu ions with energies between 10 and 100 eV for angles of incidence between 0 and $90°$. The sticking probability increases above $60°$ for ion energies between 15 and 50 eV, a regime important for PVD. If trapping occurs, an incident Cu atom will be more likely to collide with vicinal growth layers or adatom clusters, and the resulting sputtering and transport of material may be important to the growth of the feature.

II. SIMULATION METHOD

For our MD simulations, we used an embedded atom method (EAM) interatomic potential[10] in which a pair potential is augmented with a local density-dependent term. This form of potential has had considerable success in describing face-centered cubic (fcc) transition metals. The Cu potential used here[11] was fit to experimental properties of the bulk solid and gas-phase diatomic molecule. Sputter yields for normal incidence of Ar^+ on Cu(111) up to 250 eV and for Cu^+ on Cu(111) up to 100 eV computed with MD simulations using this potential[1] were in very good agreement with experiment.[12] The MD simulation procedure employed was similar to the one designed for the reactive ion etching of Si by Cl ions.[13] The MD simulation cell was comprised of 972 Cu atoms arranged as an fcc crystal of $12 \times 9 \times 9$ atoms (x,y,z) with periodic boundary conditions imposed along the x and y axes (periods = 23.00 and 26.56 Å, respectively) and a free (111) surface normal to the z axis. The bottom two layers (216 atoms) were rigidly fixed at all times. After equilibrating the free Cu(111) surface to $T = 300$ K, a Cu atom with the desired incident energy and impact angle was positioned randomly in x and y above the surface and just inside the interaction distance for the potential. The azimuthal angle was also chosen randomly.

Interatomic forces were computed from the total energy and the equations of motion were integrated using the leap-frog Verlet method.[14] The total integration time of 5 ps was sufficient to ensure that every impact atom either desorbed or adsorbed. For each impact angle and energy, 150 events were run. Ideally, one would prefer to use very large simulation cells so that the impact atom always interacted with a pristine portion of the local surface at every oscillation, but this was not feasible due to computational limitations. Typical impact velocities (~ 100 Å/ps for 35 eV) were such that a trapped impact atom crossed the simulation cell many times, as a result of the periodic boundary conditions, before coming to rest. As the impact atom slowed down, the kinetic energy transferred to the cluster caused the temperature to increase with time during the trajectory. With this system size, we were unable to find a viable method for thermostatting the cluster to prevent or ameliorate this effect, but, as

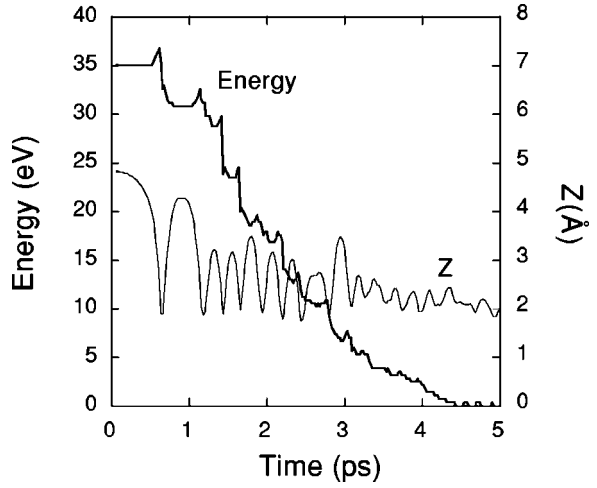

FIG. 2. Energy and height (z) above the surface as a function of time for a 35-eV Cu atom incident at 90 ° with respect to normal on Cu(111). The top layer of Cu atoms is at $z=0$. The abrupt energy losses correlate with the minima in *z*.

discussed below, we were able to quantify the effect of the temperature of the substrate.

III. RESULTS

Many individual trajectories were examined to gain insight into the trapping and energy dissipation processes and how they are related. In the following discussion, the term ''incidence angle'' will refer to the angle between the velocity vector of the atom and the surface normal when it just reaches the potential cutoff distance. The temporal history of the energy and height above the surface for a 35 eV Cu atom incident on a Cu(111) surface at 300 K is shown in Fig. 2. The initial height above the surface was 4.8 Å, just inside the cutoff distance for the potential, and the angle of incidence was 90 ° with respect to normal. As it begins to interact with the surface, the atom gains approximately 2.5 eV of kinetic energy normal to the surface (the well depth of the atom-surface interaction potential) resulting in an impact angle of ~85 °. Depending on the energy, there is a finite probability for trapping in the mean attractive field after the initial impact. The atom will be trapped if the *z* momentum it receives at impact is insufficient for escape from the surface potential well. Conversely, if the collision with the surface imparts enough *z* momentum to escape the approximately -2.5 eV well, it will desorb.

When trapped, as was the case in Fig. 2, the atom oscillates in the *z* direction, periodically impacting the surface every ~0.2 ps, at the same time traversing the surface in *x* and *y*. We shall refer to the first and subsequent encounters the atom makes with the surface at each oscillation as primary and secondary, respectively. In Fig. 2, for the first 3 ps, we see that the atom loses energy by abrupt changes that correlate with the minima of the oscillations, i.e., the impact (the abrupt regime). During this initial time (the first 7 oscillations), energy is dissipated at about 4 eV per oscillation, and the overall loss rate appears to be approximately linear. Later in the trajectory, between 3 and 4.5 ps, the amplitude of motion in *z* is less, and the energy loss is much smoother (the smooth regime). It is still nearly linear but the rate is less, about 2 eV per oscillation. Several features of the *z* trajectory in Fig. 2 distinguish the two regimes. The minima are quite sharp in the abrupt regime but more rounded in the smooth regime, and the oscillation height in the smooth regime is significantly less than in the abrupt regime. The minimum *z* values are about the same for both the smooth and abrupt regimes, presumably due to the steep inner wall of the potential.

From the examination of trajectories at various energies and azimuthal angles, we believe that the occurrence of the two regimes correlates with the oscillation height of the atom. For secondary impacts, the impact angle is determined by the ratio of normal to transverse momenta. The maximum height of the oscillation determines the amount of potential energy that is converted to kinetic energy, which defines the normal momentum just before impact. Lower amplitude oscillations lead to shallower impact angles producing weaker interactions with the surface and a smoother energy loss. Higher amplitude oscillations correlate with greater momentum exchange. The energy loss shown in Fig. 2 begins with the abrupt regime and then changes to the smooth regime at about 3 ps, and, overall it does not appear linear. In other simulations, however, we have noted that the energy loss can begin in the abrupt regime, transition to the smooth and then return to the abrupt, perhaps alternating several times. For all of the cases we have examined which exhibit trapping, it appears that, over the entire trajectory, a constant energy loss rate is a reasonable approximation. For purposes of constructing a simple phenomenological model (described below), we assume that, for secondary impacts, the energy loss mechanism is described by a single loss rate that is the appropriate average over both the abrupt and smooth regimes. This implies that dE/dx is inversely proportional to the velocity, $1/v$, or $E^{-1/2}$. In contrast, Dodson[3] found that dE/dx was linear with energy for Si trapping on the Si(111) surface. However, these findings may not be inconsistent; plots of the two expressions look quite similar. When the energy loss versus distance for a trapped trajectory is evaluated over a limited energy range, the $E^{-1/2}$ behavior could easily be interpreted as linear in *E*.

The case shown in Fig. 2, a 35 eV atom incident at 90 °, illustrates capture, i.e., the atom becomes trapped, dissipates nearly all of its energy and then adsorbs. Since there is a finite probability that the atom can desorb during each oscillation, a more likely outcome for these conditions is that the impact atom becomes trapped for only a few oscillations and then desorbs. This occurs if, during a secondary impact, the atom receives sufficient *z* momentum to escape the mean attractive potential of about 2.5 eV. Figure 3 shows a representative distribution of ''normal energies,'' E_z, for secondary impacts at 35 eV. For these simulations, the starting height was 2.8 Å, a value found to be typical for secondary oscillations, and the angle of incidence was 90 °, consistent with being at the top of a trapped trajectory. The criterion for desorption is defined as

$$E_z = p_z^2/2m \geq 2.5 \text{ eV}, \tag{1}$$

where p_z is the momentum in the z direction and *m* is the mass of the atom. To determine the desorption probability associated with a single impact, a series of MD simulations

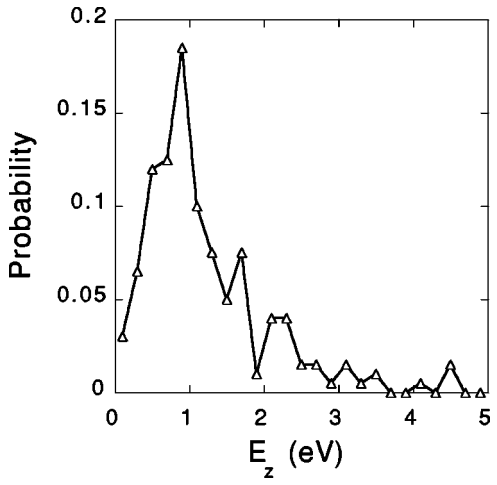

FIG. 3. Distribution of the ''normal energy'' ($E_z = p_z^2/2m$) following a secondary impact of a 35-eV Cu atom on a Cu(111) $T = 300$ K surface. Cu atoms were incident at 90° with respect to normal, 2.8 Å above the top layer of atoms, randomly positioned in x and y. 200 trajectories were run.

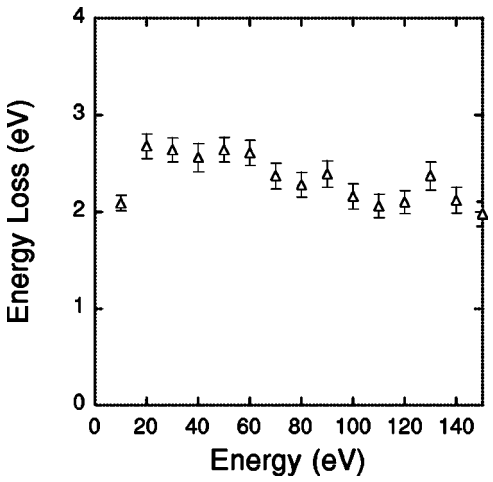

FIG. 5. Energy loss for a single oscillation after a secondary impact on a $T = 300$ K, Cu(111) surface. Each data point represents 150 impact events; error bars are one standard deviation of the mean.

over a range of energies (10 to 150 eV) were run, integrating the trajectory for only the primary impact (starting height = 4.8 Å) or a single secondary oscillation (starting height = 2.8 Å). We shall refer to these probabilities as primitive desorption probabilities. The trajectories were integrated for exactly one oscillation, i.e., to the subsequent maximum z value or until the atom desorbed. E_z was computed at each time step and the maximum value was saved. At each energy, 150 trajectories were run and the desorption probability was computed as the fraction of cases for which the criterion in Eq. (1) was satisfied. Note that this procedure results in a suitable average over both the abrupt and smooth regimes. These results are shown in Fig. 4 with a third order polynomial fit to the data. From the same set of simulations, for

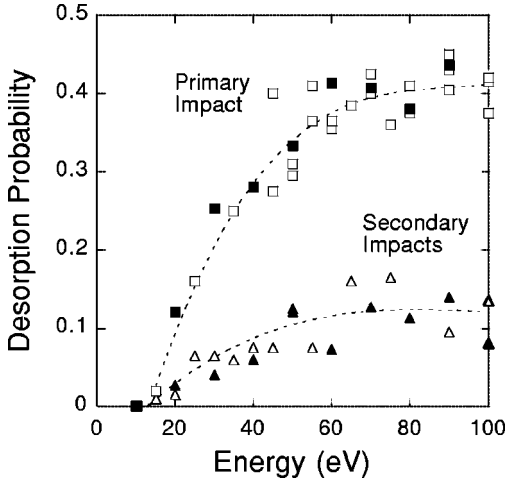

FIG. 4. Desorption probability versus energy for primary and secondary impacts at 90° incidence with respect to normal on a $T = 300$ K, Cu(111) surface (open symbols) and Cu(001) surface (solid symbols). Primary impact trajectories started just inside the potential cutoff distance, 5 Å, and secondary trajectories started at $z = 2.8$ Å, a typical oscillation height. Third order polynomial fits to the Cu(111) data are shown as dotted lines. Initial impacts were fit out to 100 eV, secondary impacts to 150 eV.

impact energies between 20 and 100 eV at 90° incidence, the average energy losses for primary and secondary impacts were determined to be 4.5 ± 0.3 and 2.5 ± 0.2 eV, respectively. Essentially identical values for the desorption probabilities were also obtained for a Cu(001) surface at 300 K. This average energy loss for secondary impacts is remarkably close to the surface potential well depth (which actually varies between 2.15 and 2.5 eV with position), and it is tempting to ask if they are related. We can make no such claim in this paper, but a cursory examination of a trapped trajectory for Pt/Pt(111) (for which the well depth is ~4 eV) indicates that the energy loss may indeed be related to the potential energy well depth. As will be described below, these primitive probabilities and the energy loss rate will be the basis for a phenomenological model for the sticking probability. The energy loss rate for secondary impacts, shown in Fig. 5, is nearly independent of ion energy down to 20 eV. Energy loss rates for primary impacts at 80° and 90° incidence are shown in Fig. 6. While the loss rate for 90° incidence is approximately independent of ion energy, this is not the case for 80° incidence, due to the normal component of the momentum that increases with energy. The standard deviation of the distribution of the energy loss at each energy was quite large, ~2 eV, and comparable for both 80 and 90°. Error bars in Fig. 6, shown only for the 90° incidence case, are one standard deviation of the mean.

We now present a simple phenomenological model to describe the sticking probability. Using the primitive desorption probabilities and average energy loss rates, the sticking probability for an impact atom at an arbitrary energy may be computed numerically as:

$$P_{stick} = \prod_{i=1}^{n} [1 - P_{desorb}(E_i)], \tag{2}$$

$$E_i = E_0 - i\Delta E, \tag{3}$$

where $P_{desorb}(E)$ is the desorption probability per impact taken from the polynomial fit in Fig. 4, E_o is the initial energy, ΔE is the energy loss at impact or per oscillation,

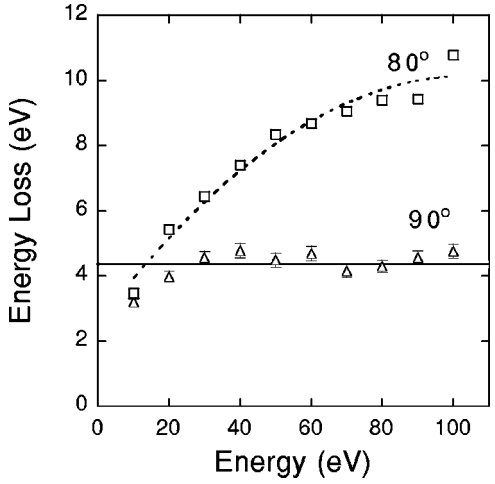

FIG. 6. Energy loss rate (per impact) for primary impacts on Cu(111) at $T=300$ K at angles of incidence of 80° (dashed line) and 90° (solid line). Each data point represents 150 impact events; error bars are one standard deviation of the mean. The dashed line is a second order polynomial fit to the data, $\Delta E=2.5+0.145E-0.00067E^2$.

and i is the number of oscillations. These equations were solved iteratively from the initial energy down to 10 eV, the energy at which the desorption probability essentially goes to zero (see Fig. 4). Sticking probabilities calculated with this phenomenological model are compared to those obtained from full MD simulations in Fig. 7. For 90° incidence, the primary and secondary impact energy losses used were the calculated values of 4.5 and 2.5 eV, independent of impact energy. For 80° incidence, the energy loss per secondary impact was 2.5 eV, and for primary impacts computed as $\Delta E=2.5+0.145E-0.00067E^2$ (the polynomial fit shown in Fig. 6). The predicted sticking probability is in good qualitative agreement with the full MD results. Including the slight linear dependence of energy loss with energy for secondary impacts, seen in Fig. 5, in the phenomenological model has a negligible impact on this agreement.

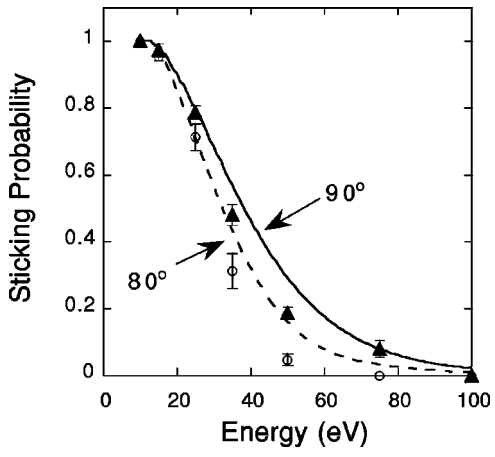

FIG. 7. Comparison of the sticking probability computed by phenomenological model in Eqs. (2) and (3) for angles of incidence of 90° (solid line) and 80° (dotted line), and values from full MD simulations at 90° (solid triangles) and 80° (open circles). For secondary impacts, the energy loss per impact was constant, 2.5 eV. For primary impacts, the energy loss per impact at 90° was 4.5 eV, independent of energy, and at 80° computed from $\Delta E=2.5+0.145E-0.00067E^2$. Error bars are one standard deviation of the mean.

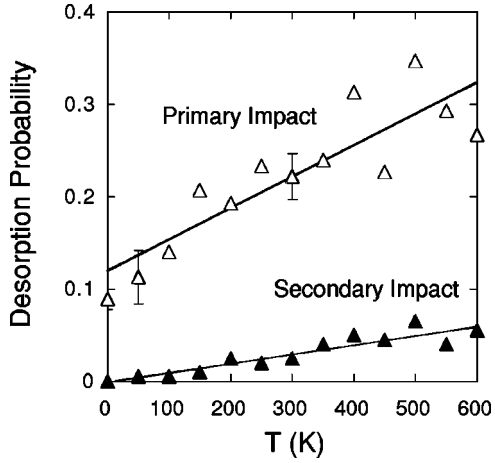

FIG. 8. Dependence of the desorption probability on surface temperature for a 35-eV Cu atom incident on a Cu(111) surface at 90° incidence with respect to normal. Each data point is the average of 150 cases randomly positioned in x and y with random azimuthal angle. Representative error bars are one standard deviation of the mean. Straight lines are the least squares fits, $y=0.12+0.00034x$ and $y=0.00001+0.0001x$.

As mentioned in Sec. II, we did not impose a thermostat on the simulation cluster during the trajectory calculations, and this resulted in the cluster heating up as the impact atom lost energy ($\Delta T\sim 360$ K for 35 eV deposited). In this respect, the phenomenological model may be more accurate than the full MD simulations since it is based on single impact MD calculations in which no abnormal heating can occur. Based on the temperature dependence of the desorption probabilities, described below, this would cause the full MD results to err on the side of a lower sticking probability and this is consistent with the disagreement seen in Fig. 7. Simulations of 35 eV impacts incident at 90° for surface temperatures between 0 and 600 K, shown in Fig. 8, indicate that the desorption probability depends on the temperature of the substrate. The desorption probabilities increase approximately linearly with temperature with slopes of 0.00034 and 0.0001 K^{-1}, for primary and secondary impacts, respectively. However, the average energy loss for secondary impacts did not change with surface temperature. That the desorption probability for both primary and secondary impacts is linear with temperature is surprising, and we can offer no explanation. We note, however, that the mean square surface roughness must increase linearly with temperature according to the Debye-Waller equation, $3/2\ KT=1/2m\omega^2\langle u^2\rangle$, where m is the mass of the atom, ω is the vibration frequency and $\langle u^2\rangle$ is the mean-square displacement. Below 50 K, the desorption probability for secondary impacts is essentially zero; at $T=0$ K, the desorption probability for secondary impacts at 35 eV is <0.001. When the phenomenological model was modified to include surface heating and temperature dependent desorption probabilities were used in Eq. (2) (assumed valid for all energies), the agreement between the phenomenological model and the full MD results improved significantly. The sticking probability predicted by the phenomenological model was within one standard deviation of

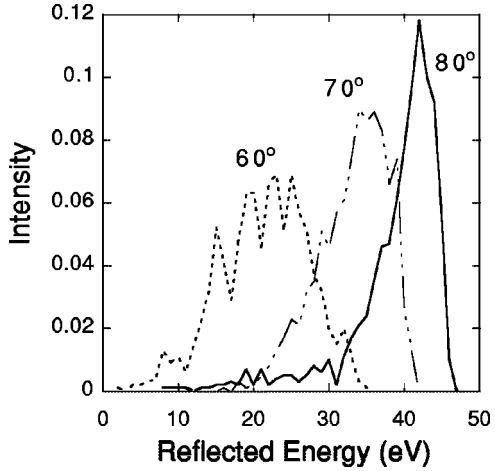

FIG. 9. Reflected kinetic energy distribution for 50-eV Cu ions on a 300-K Cu(111) surface for three angles of incidence as predicted by full MD simulations. The structure in the 60 ° distribution is not statistically significant.

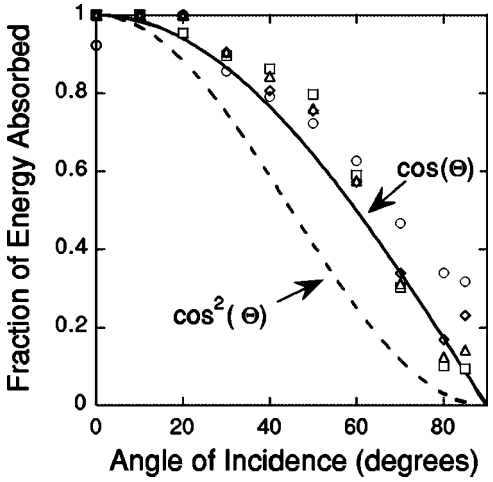

FIG. 10. Average fraction of energy dissipated to surface versus angle of incidence for Cu atoms incident on a $T=300$ K Cu(111) surface at energies of 25 eV (circles), 50 eV (diamonds), 75 eV (triangles), and 100 eV (squares). Each point is the average of 150 trajectories. For comparison, lines for $y = \cos(\Theta)$ and $y = \cos^2(\Theta)$ are also shown.

the mean for five of the six full MD values. We believe that the overall agreement validates the phenomenological model as an accurate description of the trapping-desorption process.

An analytic expression for the total distance that a trapped atom travels before coming to rest can be derived from Eqs. (2) and (3) in the continuous limit by casting the energy loss equation in Eq. (3) as a temporal derivative rather than an energy loss per oscillation. Noting that the velocity is proportional to the square root of the energy, the total distance traveled, R_{tot}, is just the time integral of $[2E(t)/m]^{1/2}$. The result is

$$R_{tot}=a(E_0)^{3/2}, \tag{4}$$

where R_{tot}(Å) is the total distance traveled from the point of primary impact, E_0 is the initial energy (eV), and $a = 1.03$ Å/eV$^{3/2}$. For the Cu/Cu(111) system, the total distance predicted by this expression evaluated at 35 eV is 169 Å, which is about 17% less than the mean value obtained from MD simulations, 203 ± 3.5 Å.

The predicted energy loss that occurs while the atom is trapped on the surface is manifested in the reflected kinetic energy distribution. Examples are shown in Fig. 9 for 50 eV Cu atoms incident at 60, 70 and 80 ° on a $T=300$ K Cu(111) surface, where each distribution is constructed from 1000 impacts. At 80 ° incidence, the reflected energy distribution has a narrow peak at about 42 eV and a pronounced foot extending from 15 to 30 eV. The foot, which is the signature of surface trapping, is due to the arbitrary energy loss that can occur before desorption depending on the number of oscillations the atom makes on the surface. The presence of a low-energy foot was also evident in the MD results obtained by Smith *et al.*[7] for 1 keV protons on Cu(111) at 86 ° with respect to the surface normal. The peak at 42 eV is due to the high probability associated with reflections occurring immediately after the 50 eV primary impact, for which the energy loss is just the normal energy component at impact. The average sticking probabilities at these angles, 60, 70, and 80 °, were 0.04, 0.03, and 0.09, respectively. The reflected energy distributions from both Cu(111) and Cu(001) surfaces were compared for 50 eV atoms at 85 ° incidence and were found to be essentially identical.

A plot of the average fraction of energy absorbed by the surface versus angle of incidence for reflected atoms is shown in Fig. 10. Fractions of energy absorbed were calculated for incident energies of 25, 50, 75 and 100 eV, and angles of incidence up to 85 °. The average fraction of energy absorbed at each angle of incidence, Θ, in Fig. 10, scales approximately as cos(Θ). This is surprising since the ''normal'' energy scales as $\cos^2(\Theta)$, and one might expect that only this component would dissipate at impact. However, more than the initial normal component of energy can be transferred to the surface. As shown in Fig. 6, impacts with sufficiently high normal momentum (determined by both the angle of incidence and impact energy), can cause the atom to dissipate some fraction of the parallel energy

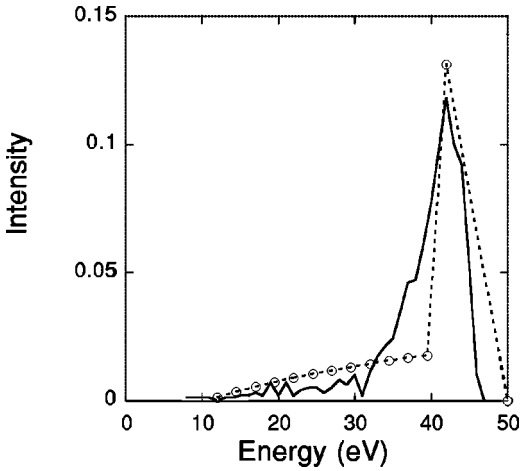

FIG. 11. Reflected kinetic energy distribution for 50-eV Cu ions at 80 ° incidence on a 300-K Cu(111) surface as predicted by the phenomenological model (open circles) compared to the MD simulation result (solid line). The dashed line is added to facilitate comparison.

component during the primary impact. At grazing incidence, multiple oscillations will also serve to dissipate some of the parallel energy. For energies above 25 eV, the fraction of energy absorbed appears to be independent of incident energy and scales close to $\cos(\Theta)$ and is clearly greater than $\cos^2(\Theta)$. This is consistent with the experimental data of Winters *et al.*[15] for low energy Ar ions impacting a Pt(111), $T=800$ K surface, interacting via a Van der Waals force.[15] Their data clearly show, and they concluded, that the fraction of energy deposited to the surface obeys a $\cos(\Theta)$ dependence.

The reflected energy distribution for 50 eV atoms incident at 80° predicted by the phenomenological model [Eqs. (2) and (3)], shown in Fig. 11, is in very good agreement with the distribution obtained from the MD simulation. The curve for the phenomenological model starts at 42 eV because the initial energy loss value used in Eq. (2) was ~8 eV.

IV. CONCLUSION

The results of MD simulations of Cu atoms impacting a Cu(111) or Cu(001) surface at grazing incidence elucidate the occurrence of the trapping-desorption phenomenon, which we believe explains the unexpected upturn in the sticking probability with impact angle shown in Fig. 1. At energies up to 100 eV, an impact atom can become trapped in the mean attractive field above the surface for long times (>3 ps) while traveling large distances (>100 Å) over the surface. While the atom is trapped, it oscillates anharmonically perpendicular to the surface and loses energy in a piecewise linear fashion through interactions with the surface atoms. An examination of all of the trajectories that exhibit trapping suggests that a constant energy loss rate, dE/dt, is a reasonable approximation. The primitive desorption probabilities for both primary and secondary impacts and the average energy loss per impact have been calculated by MD simulations for impact energies up to 100 eV. A phenomenological model, using these primitive desorption probabilities and energy loss rate, predicts values for the sticking probability, the total distance traveled before adsorption, and the reflected energy distribution that are in very good agreement with full MD simulations. For impact energies above 25 eV, the average fraction of energy dissipated to the surface between impact and reflection or adsorption scales approximately with the cosine of the angle of incidence. Based on the similarity between the energy loss distributions and primitive desorption probabilities for Cu(111) and Cu(001) surfaces, we expect that the overall behavior of the two surfaces is quite similar with respect to the trapping desorption process.

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