

# Trapping and Desorption of Energetic Cu Atoms on Cu Surfaces at Grazing Incidence

David E. Hanson, Joel D. Kress, Art F. Voter, and X.-Y. Liu (Motorola)

As the semiconductor industry continues to reduce the feature size of computer chips, it is clear that a better understanding of the surface chemistry and physics is necessary to model and optimize the required manufacturing processes. Molecular dynamics (MD) simulations have proven to be a valuable tool for studying gas-surface interactions at an atomic level, and we have applied these techniques to investigate the variation in sticking probability with energy and impact angle<sup>1</sup> for an energetic metal atom impacting a surface for a variety of metals. Figure 1 shows the sticking

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probability for Cu ions incident on a Cu surface as a function of impact angle, parametric on energy. For angles of incidence (with respect to normal) up to 20°, the sticking probability is unity for all energies; the impact atom penetrates and loses all of its kinetic energy to the surface. As the impact angle increases, the probability for the impact atom to reflect increases, reducing the sticking probability. Surprisingly, for angles above 70°, the sticking probability increases with impact angle. From detailed simulations, we found that this unexpected upturn is a consequence of a surface trapping phenomena. Based on these studies, we developed a simple, two parameter phenomenological model that describes this behavior. It is relevant to semiconductor modeling because copper is typically deposited on micro circuit features for which the sidewalls are nearly parallel to the incident ion beam.

From our simulations of Cu<sup>+</sup> ions incident on a Cu crystal surface at grazing incidence<sup>2</sup>, we found that an energetic Cu

ion can become trapped by the mean attractive potential that exists above the surface. In this trapped state, the atom “bounces” along the surface dissipating its kinetic energy via inelastic collisions with the surface at a nearly constant rate, i.e.,  $dE/dt = \text{constant}$ . The energy and height above the surface for a 35-electron volt (eV) Cu atom incident on a Cu surface is shown in Figure 2. Before the atom starts to slow down, it gains approximately 2.5 eV of kinetic energy normal to the surface (the well depth of the atom-surface interaction potential). Depending on its energy, there is a finite probability for trapping after the initial impact by the mean attractive field. The atom will be trapped if

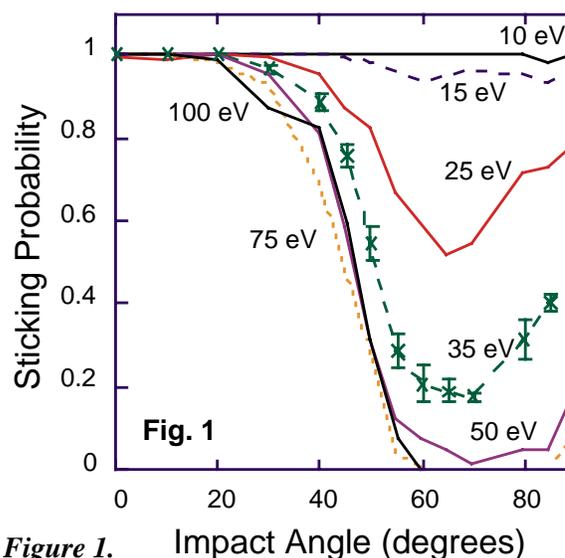


Figure 1. Impact Angle (degrees)

the vertical momentum it receives at impact is insufficient to overcome the surface potential well. Conversely, if the collision with the surface imparts enough vertical momentum, it will desorb.

When trapped, as was the case in Figure 2, the atom oscillates normal to the surface, periodically impacting the surface every  $\sim 0.2$  picoseconds (ps), at the same time traversing the surface for 100's of Ångströms (Å). For the first 3 ps, we

see that the atom loses energy in abrupt changes that correlate with the minima of the oscillations. Later in the trajectory, between 3 and 4.5 ps, the amplitude of the vertical motion is less, and the energy loss is much smoother. It is still nearly linear but the rate is significantly less. On average, we find that the energy loss rate is quite linear down to 10 eV.

The case shown in Figure 2 illustrates capture, i. e., the atom becomes trapped, dissipates its energy, and then adsorbs. Since there is a finite probability that the atom can desorb at each oscillation, a more likely outcome for these conditions is that the impact atom becomes trapped for only a few bounces and then desorbs. This occurs if the atom receives sufficient vertical momentum to escape the mean attractive potential of about 2.5 eV. To determine the desorption probability associated with a single impact, a series of simulations over a range of energies (up to 150 eV) were run. The trajectories were integrated for exactly one oscillation, or until the atom desorbed, and the maximum “normal” energy  $E_z = P_z^2/2m$  was calculated. The desorption probability was computed as the fraction of cases for which  $E_z$  was greater than 2.5 eV, the attractive potential well depth.

These primitive probabilities and the constant energy loss rate are the basis for a phenomenological model for grazing surface interactions. The sticking probability for an impact atom at an arbitrary energy may be computed numerically as  $P_{stick} = \prod_{i=1}^n (1 - P_{desorb}(E_i))$ , where  $E_i = E_o - i\Delta E$ ,  $P_{desorb}(E)$  is the desorption probability per impact as calculated above,  $E_o$  is the initial energy,  $\Delta E$  is the energy loss at impact or per oscillation, 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 goes to zero. Sticking probabilities calculated with this phenomenological model are compared to those obtained from full molecular dynamics simulations in Figure 3. The predicted sticking probability is in good agreement with the full simulation results, which, we believe, 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 the

above equations in the continuous limit by casting the energy loss as a temporal derivative. The result is  $R_{tot} = a(E_o)^{3/2}$ , where  $E_o$  is the initial energy (eV) and  $a = 1.03 \text{ \AA}/\text{eV}^{3/2}$ . The total distance of 169 \AA predicted by this expression evaluated at 35 eV, is in good agreement with the mean value obtained from full simulations,  $203 \pm 3.5 \text{ \AA}$ .

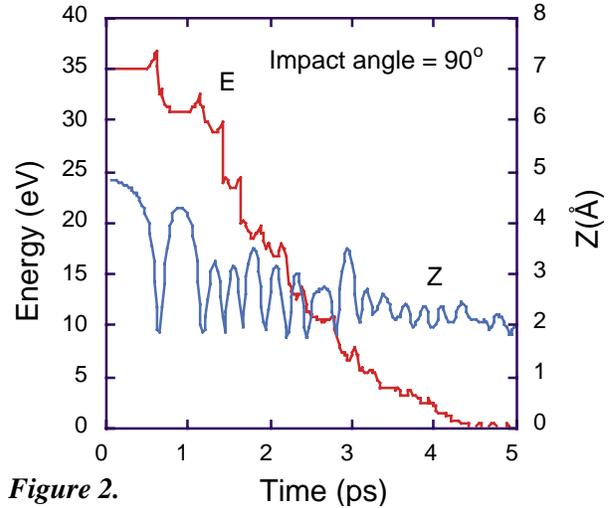


Figure 2.

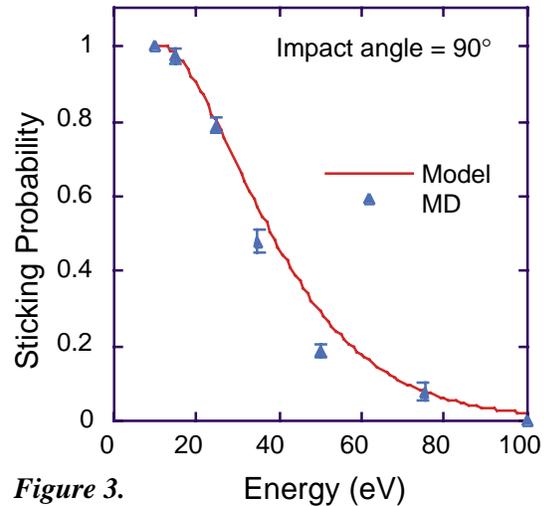


Figure 3.

[1] D. G. Coronell et al., *Appl. Phys. Lett.* **73**, 3860 (1999), and J. D. Kress et al., *J. Vac. Sci. Tech (A)* **17**, 2819.

[2] D. E. Hanson, A. F. Voter, J. D. Kress, and X.-Y. Liu, *Phys. Rev. B* **60**, 11723 (1999).