Eur. Phys. J. D **24**, 319–321 (2003)
DOI: 10.1140/epjd/e2003-00152-3

THE EUROPEAN PHYSICAL JOURNAL D

Molecular dynamics study of metallic surface smoothing by cluster impact

F. Palacios[a], R. Méndez, and M.P. Iñiguez[b]

Departamento de Física Teórica y Atómica, Molecular y Nuclear, Universidad de Valladolid, Spain

Received 10 September 2002
Published online 3 July 2003 –

Abstract. In this work, Molecular Dynamics (MD) simulations are performed to study the smoothing of a rough Al(111) surface by means of metal cluster impact. A projectile Al_{13} cluster impinges on an island-shape defect supported over the surface at incident angles of 15°, 45° and 90°, and with the initial kinetic energy being varied from 1 to 40 eV/at. Depending on the angle and the initial kinetic energy, several phenomena take place, from projectile sticking and island flattening to fragmentation and sputtering with substrate damage for the largest energies.

PACS. 36.40.-c Atomic and molecular clusters – 68.35.Bs Structure of clean surfaces (reconstruction)

1 Introduction

Cluster beams impacting on surfaces produce much stronger effects than ion beams for the same total energy, the reason being the much higher energy density and stopping power. This powerful technique has been used to produce thin films [1], to promote sputtering [2,3], or to smooth rough surfaces [4,5] among others. Some of them are addressed in this work. Very different behaviours are expected depending on the type of bonding involved in both, the projectile and the substrate. For example [4,5], the projectile can rebound or can stick to the surface, the last one being more common for metallic elements. Although most of the cluster impact simulations have been done at perpendicular incidence, the importance of the incidence angle for the lateral atomic displacements and its relation to surface smoothing has been stressed [4]. We study here the dependence of the smoothing process with the incidence angle and the projectile kinetic energy. The energetic ranges for different outcomes after the impact are analyzed. We obtain that small incidence angles promote an important lateral sputtering effect on the atoms in the protuberances of the rough surface. This fact and the lower damage of the substrate, can make low angle cluster impact a useful tool for cleaning and smoothing surfaces.

2 Model

A parallelepipedic block for the Al(111) surface is built with atomic layers each one containing 1000 atoms. The three bottom layers are fixed, the next one is frictive [6] and the rest of the layers are treated by constant energy MD. For the higher energies the number of constant energy layers is increased to assure a correct modelling of the substrate. The substrate is initially thermalized at $T = 0$ K and the simulation is runned up to 10 ps which is enough for the main features to take place. Surface roughness is modelled by a cluster island whose atomic configuration is obtained by relaxing a free 55 atom Al cluster on top of the surface. The projectile, a 13 atom Al cluster, impinges the substrate at an incidence angle determined by the line joining the center of masses of the projectile and the island. At the initial time the distance between those two center of masses is 15 Å.

The atomic interactions are modelled by a many-body semiempirical potential rooted on the tight-binding formalism [7]. The total potential energy for a N atom system is given by

$$V = \frac{1}{2}\sum_{i=1}^{N}\left[\sum_{j=1}^{N} A\mathrm{e}^{-p(r_{ij}/r_0-1)} - \left(\sum_{j=1}^{N}\xi^2\mathrm{e}^{-2q(r_{ij}/r_0-1)}\right)^{1/2}\right] \quad (1)$$

with $j \neq i$ and r_{ij} being the distance between atoms i and j. The first term is a repulsive pair potential and the second is an attractive many-body band-energy contribution. The parametrization used was obtained by fitting to properties of the pure metal Al [8]. Only interactions up to fifth nearest neighbours were considered in those fittings, thus a corresponding cutoff radius for the potential has

[a] e-mail: palacios@fcualab.fam.cie.uva.es

[b] Work supported by DGES (Grant PB98-0368).

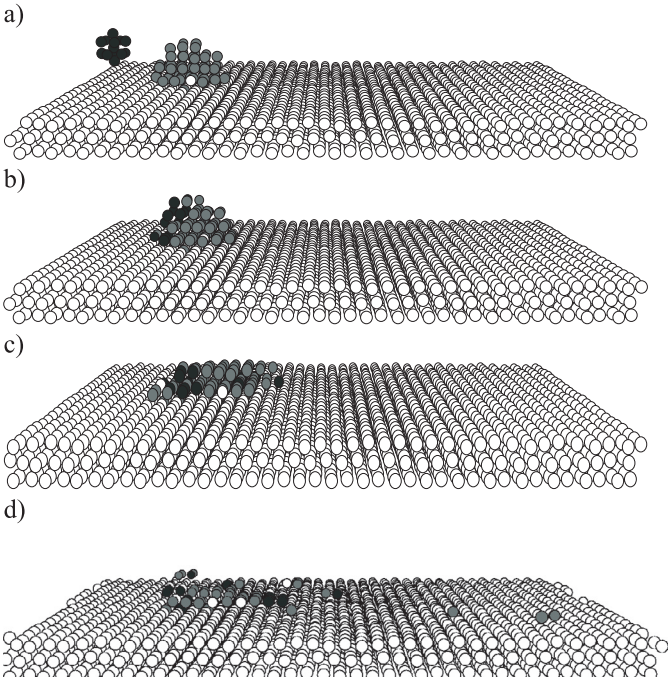

Fig. 1. Snapshots at initial time (a) and at 5 ps for several energies: (b) 1 eV/at, (c) 5 eV/at and (d) 20 eV/at.

been used to save computation time. It is evident that, due to the nature of the potential which does not consider explicitly the electrons, the charge rearrangements caused by the impact are discarded in this work.

We have used this potential in previous works on cluster deposition and cluster-cluster collision simulations [9–12]. Those references are useful to compare with the present work.

3 Results

The projectile energy plays a determinant role in the further evolution of the system as Figure 1 shows. The starting $t = 0$ and $t = 5$ ps configurations are pictured for an incidence angle of 15° and several energies. The most striking configuration changes occur before this time, the temperature in the impact zone reaches a sharp peak and falls down very quickly after that. At longer times much more slow thermally driven atomic position changes take place,which were studied in a larger simulation of cluster deposition events [12]. Substrate temperature was found to play also an important role in the smoothing of metallic islands in that work.

As can be noticed at low energies (1 eV/at), time evolution of the system is characterized by the production of a larger island as a result of the projectile sticking. The smoothing is negligible and the number of atomic layers is the same as in the original supported island (Fig. 1b). The energy is not enough to promote atomic interdiffusion between projectile and island atoms. However, increasing the kinetic energy (Fig. 1c) allows the flattening of the island from its four initial monolayers to a two monolayers

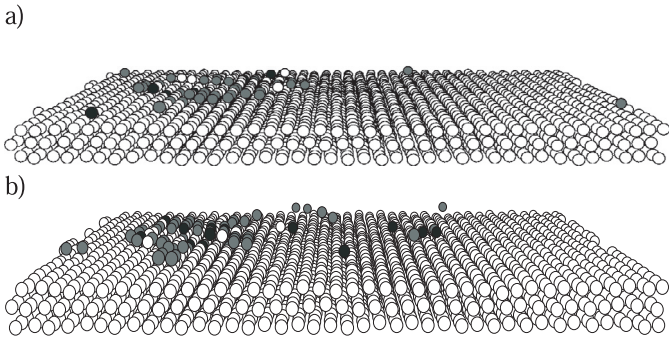

Fig. 2. Snapshots at 5 ps and 20 eV/at for (a) 45° and (b) 90°.

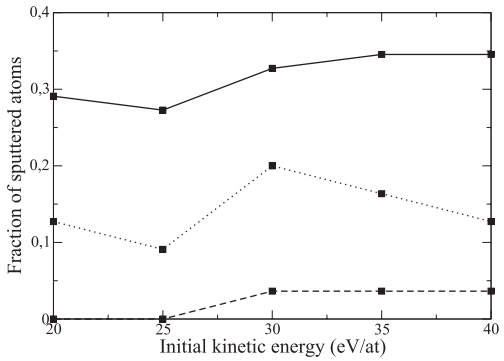

Fig. 3. Sputtering yields for 15°, 45° and 90°. Upwards curves for decreasing angle.

structure. Higher energies produce a total flattening and, as a consequence, the initial defect becomes a fragmented monolayer structure supported on the substrate (Fig. 1d). In all cases, substrate damage is very small. An additional factor that influences smoothing is the sputtering of the island atoms. Figure 2 shows the island configurations at 5 ps corresponding to the energy of 20 eV/at at incidence angles of 45° and 90°. It is clear, by comparison to Figure 1d, that the size of the final disgregated island is lower for small incidence angles due to an enhanced lateral sputtering mechanism. This sputtering mechanism was also observed for cluster impacts onto flat surfaces [13].

For a given projectile energy the number of sputtered atoms increases for smaller incidence angles, see Figure 3, being negligible for perpendicular incidence in this range of energies.

This suggests that low incidence angle cluster impact can be an efficient method for surface cleaning and desorption, taking into account that substrate damage is not very important at low angles.

We can compare the outcome of cluster-cluster collision events [9] with the phenomena present in this work, where the substrate also plays an important role. A very low energy of 1 eV/at was found there to be enough for melting the fused cluster formed after the collision. Here, as the substrate absorbs a part of the impact energy, the supported island is never in a molten state. For the same

reason, the island fragmentation and the emission of atoms and small fragments is more important in free cluster-cluster collisions.

4 Conclusions

In this work an analysis of the interaction of a free cluster impacting at an island surface defects is studied. Several physical and geometrical parameters play an important role in further evolution of the system.

Initial kinetic energy of the projectile has a relevant influence in the flattening of the final defect structure on the surface, promoting atom mobility when that energy is enough.

On the other hand the incidence angle influences the sputtering rate. Simulations showed that for small incidence angles the fraction of sputtered atoms was bigger than for normal incidence. This suggests low angle incidence impact can be suitable for smoothing and cleaning surfaces.

It is also expected that chemical nature of target and projectile atoms modify the behaviour of the system as could be noticed from cluster impact and cluster-cluster collisions simulations [9–11] where changing this nature alters later system evolution.

References

1. H. Haberland, Z. Insepov, M. Moseler, Phys. Rev. B **51**, 11061 (1995)
2. S. Bouneau, A. Brunelle, S. Della-Negra, J. Depauw, D. Jacquet, Y. Le Beyec, M. Pautrat, M. Fallavier, J.C. Poizat, H.H. Andersen, Phys. Rev. B **65**, 144106 (2002).
3. T.J. Colla, H.M. Urbassek, Nucl. Instrum. Meth. B **164**, 687 (2000)
4. M. Moseler, O. Rattunde, J. Nordiek, H. Haberland, Nucl. Instrum. Meth. B **164**, 522 (2000)
5. Chang-Koo Kim, Nawoyuki Kubota, D.J. Economou, J. Appl. Phys. **86**, 6758 (1999)
6. S. Nose, J. Chem. Phys. **81**, 511 (1984)
7. R.P. Gupta, Phys. Rev. B **23**, 6265 (1981)
8. F. Cleri, V. Rosato, Phys. Rev. B **60**, 2908 (1999)
9. F.J. Palacios, M.P. Iñiguez, Nucl. Instrum. Meth. B **196**, 253 (2002)
10. F.J. Palacios, M.P. Iñiguez, M.J. López, J.A. Alonso, Phys. Rev. B **62**, 16031 (2000)
11. F.J. Palacios, M.P. Iñiguez, M.J. López, J.A. Alonso, Comp. Mat. Sci. **17**, 515 (2000)
12. F.J. Palacios, M.P. Iñiguez, M.J. López, J.A. Alonso, Phys. Rev. B **60**, 2908 (1999)
13. Z. Insepov, I. Yamada, Nucl. Instrum. Meth. B **99**, 248 (1995)