INFLUENCE OF THE TIP-SUBSTRATE ADHESION AND SUBSTRATE ORIENTATION ON THE RESPONSE OF CU MONOLAYERS TO NANOINDENTATION AND NANOSCRATCHING.

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The developing of Nanotechnologies requires further research on Nanomechanics because of size-dependent phenomena at sub-micron level. In this sense, Nanocontact phenomena and friction at nanometric scale are key subjects. In this field, embedded atom method (EAM) and other molecular dynamics (MD) techniques help to characterise the mechanical behaviour of this kind of nanostrucures.

We have performed MD simulations of nanoindentation and nanoscratching of Cu crystals on {001} and {111} surfaces using the EAM [1, 2], with an appropriate potential for Cu [3]. For simulating high adhesion conditions, an artificially rigid tip made of Cu atoms with orientation matching that of the substrate (very high adhesion) or unmatching it (*i.e.*, {111} facing {001} and *vice versa*) has been employed. For low adhesion simulations, the tip has been made of a rigid FCC material of the same parameter as Cu but interacting with the substrate with a very strong repulsive potential [4].

The simulated nanolayers are 7.2×7.2×7.2 nm^3. The atoms at the bottom of the layer are fixed. Periodic boundary conditions are applied along *x* and *y*. The nanoindenter is a sphere of ∅5.8 nm. All the atoms of the indenter are fixed to make it rigid. The simulations are carried out at 300 K. The Nosé-Hoover thermostat [5, 6] has been implemented for controlling the temperature of the system. The time step used in these simulations is 2.5 fs. In the simulations, the indenter is first moved at 80 m/s along *z* to indent the surface. After a penetration of 1 nm, the indenter moves along *x*, at the same speed, to scratch the surface.

Figure 1 shows the initial configuration of the systems. During the indentation and the scratching processes, the forces needed to move the indenter are stored. Figure 2.a and 2.b show the evolution of F_x and F_z during the simulations, once the indentation step is finished. The adhesion between the layer surface and the indenter is given by the ratio of F_x and F_z, *i.e.*, the friction coefficient μ (Fig. 3.a and 3.b). The results show a strong influence of both the adhesion and the orientation of the substrate crystals on the friction coefficient and on the subsurface structural modifications. For the strong repulsive potential, we obtain the lower friction coefficient, independently of the substrate orientation. There are few interactions between the indenter and the nanolayer, and the surface modifications appear in the outermost atomic layers (Fig. 4.a and 4.b). On the other hand, we find a very strong adhesion in the Cu-Cu contact, and particularly for the combination 001×001. As observed in Fig. 3.a, several stick-slip events take place during the simulation. The structural modifications produced in the cases with the indenter oriented along {001}, reach the innermost part of the layer (Fig. 4.c and 4.d). When the indenter is oriented along the {111} direction (Fig. 4.e and 4.f), the system does not show as much activity in terms of dislocation emission, as in the other orientation.

References:

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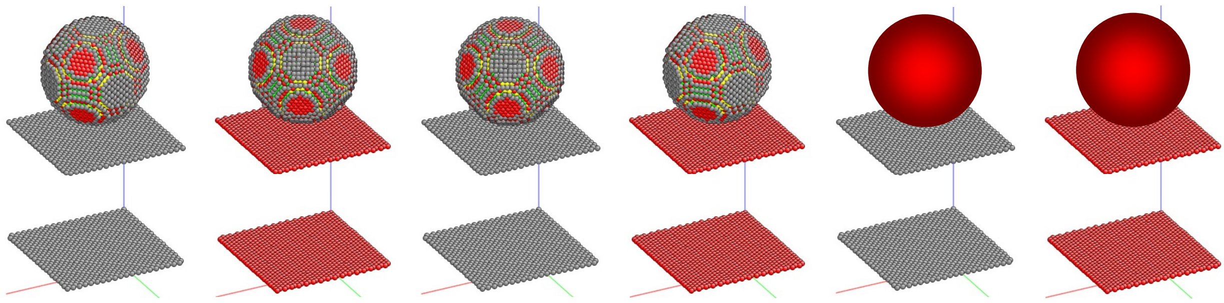
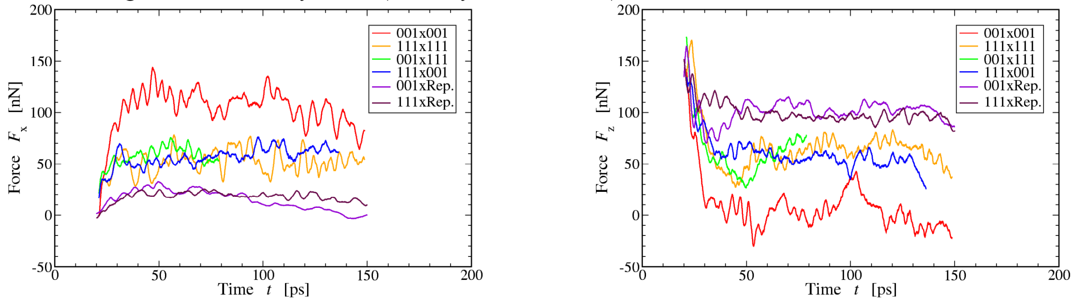
Figures:



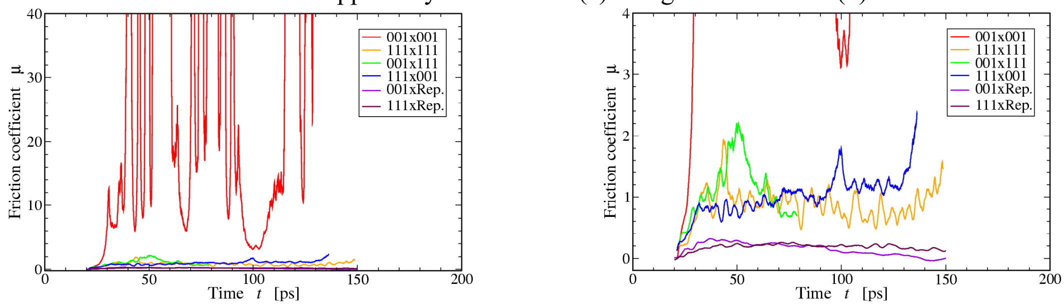
001×001 111×111 001×111 111×001 001×REP 001×REP

Fig. 1. Initial configuration of the systems (nanolayer + indenter) simulated.



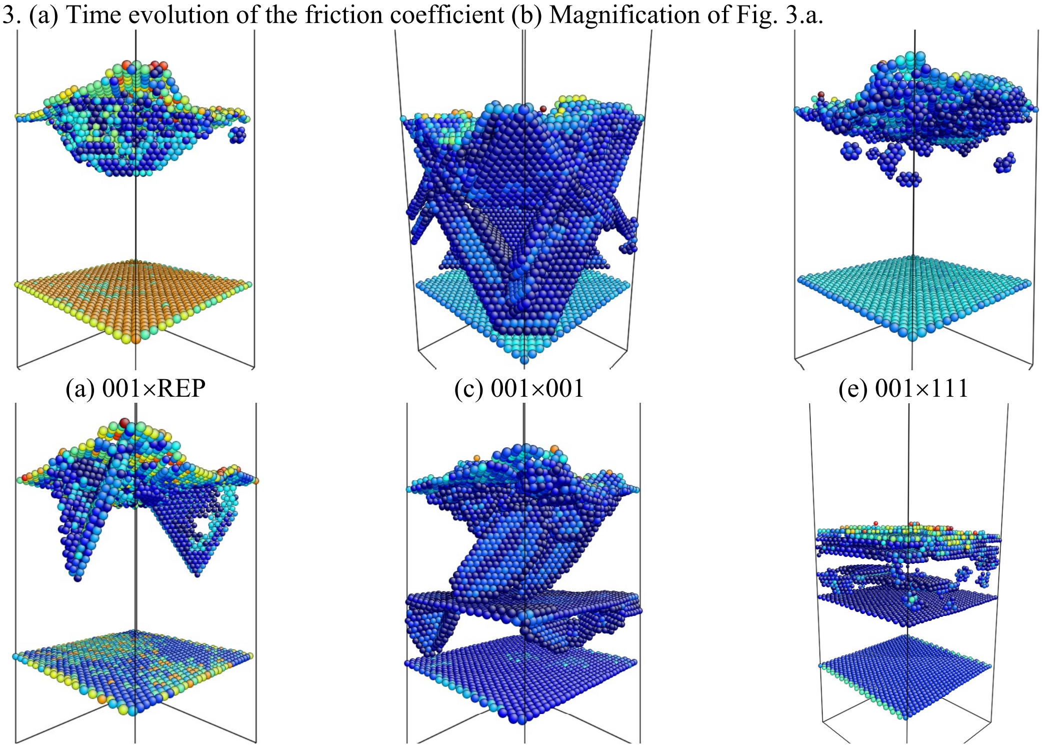
(a) (b)

Fig. 2. Time evolution of the force applied by the indenter (a) along the *x*-axis and (b) the *z*-axis.



(a) (b)

Fig. 3. (a) Time evolution of the friction coefficient (b) Magnification of Fig. 3.a.



(a) 001×REP (c) 001×001 (e) 001×111

(b) 111×REP (d) 111×001 (f) 111×111

Fig. 4. Configuration of the system when t=80 ps.