Atomistic simulation on the sliding of a rigid indenter over aluminum with crystalline defects

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1. Introduction

This work presents a molecular dynamics (MD) study of contact, indentation and dry sliding of a rigid flat punch indenter over a previously deformed metallic Aluminum slab body. The slab was deformed by means of a hydrostatic pressure in order to generate crystal defects. The crystal defects in the slab were quantified using a local coordination analysis of the atoms at different times of the simulation. The pre-deformed slab was then subjected to indentation and followed by slip of a planar rigid indenter. The strain hardening effects on friction and adhesion were studied, as a function of the amount of defects, by measuring the penetration force and the friction force. The results show that the adhesion force between atomic layers is affected by the crystal defects density.

2. Materials and methods

Four different models were developed, as shown in Fig. 1, each one with different initial crystalline defects and residual stress levels. The different amounts of crystalline defects were introduced by the imposition of different strains due to compression.

Each model is divided into five steps of simulation:

I. Initial assembly of the deformable block

II. Equilibrium of the system

III. Compression of the lower block

IV. Vertical motion of the rigid indenter until the penetration of deformable block over 3 atomic layers

V. Horizontal slip of the rigid indenter over deformable block

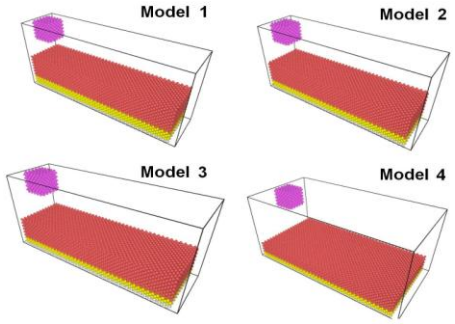

Fig. 1 - Initial dimensions of each model

Each ensemble has 17,385 atoms, arranged in a rigid indenter and a deformable slab, both constituted by FCC aluminum cells with lattice parameter 4.05Å. The slab is organized in 3 regions: two fixed atomic layers; an intermediate group, to which is applied a thermal bath condition using the Nose/Hoover thermostat algorithm; and, finally, the atoms layers that are free to move. Periodic boundary conditions with EAM potential, developed by Mishin et al. (1999) were used to describe the interactions between atoms. A cut-off radius of 6.28 Å was adopted.

3. Results and discussion

Positions and velocities of each atom were calculated. Energy, temperature, stresses and reaction forces due to penetration and slip were also obtained. A disorder parameter of the crystalline lattice is evaluated to measure the evolution of crystalline defects (Fig. 2).

Defect density affects the adhesion force between atomic layers. Defect density also affects the amount of material prow formed ahead of the indenter. Stick slip motion is also observed.

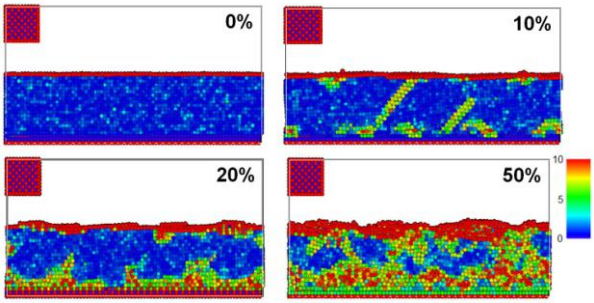

Fig. 2 - Disorder of crystalline lattice after different compression levels

4. Conclusions

The results show that the adhesion strength between atomic layers is affected by defects density in metallic crystal. Contrary to the observed in macroscopic scale, increasing the amount of defects causes a reduction in the frictional force between the contact surfaces.

5. References

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