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Molecular dynamics simulations of the nano-indentation for aluminum and copper

Xiaozhi Tang, Yafang Guo , Yu Gao

Summary

Atomistic simulations were performed to study the nano-indentation for two kinds of FCC metals, aluminum and copper. Two different deformation mechanisms were observed in our simulation under exactly the same simulation condition. An embedded atom method potential was employed for copper and a generalized form of EAM potential due to Finnis and Sinclair for aluminum. In the simulation model, the substrate was constructed with 78408 atoms in an 8I?*40I?*60I? cell, here I? means the lattice constant. The indenter was modeled by a cubic with its side length of 8a.During the simulation, the period boundary condition was applied to the (1 0 0) and (-1 0 0) direction. The indenter moved into the substrate gradually along [0 0 -1] direction with a constant speed of 22 m/s, while four bottom atomic layers in the substrate were fixed in order to avoid the displacement in loading direction. In both of the simulations, we controlled the pressure along the [1 0 0] direction to make it zero and the temperature is 5K.

In the early stage of the deformation in the copper substrate, we observed two partial dislocations separately along the [0 -1 -1] and [0 1 -1] direction emitted from the surface of the substrate just under the indenter. When the indenter moved deeper, a series of stacking faults in the (-1 1 1) plane appeared gradually and then extended to the surfaces throughout the whole substrate. However, the deformation mechanism in the aluminum substrate was totally different because no stacking faults were observed. We only found dislocations with one Burgers vector emitted from the substrate surface just under the indenter. Subsequently, dislocations moved to the surface, which finally caused a trapezoidal deformation on the substrate surface due to dislocations accumulation.

As we have known that aluminum has much higher stacking fault energy than copper. So, it's not difficult to explain that stacking faults are widely observed in copper, while only dislocations are observed in aluminum in our simulations.