Experiment and Quasicontinuum simulation of nanoindentation of single crystal copper

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Abstract: Experiment and quasicontinuum simulation [1] of nanoindentation of fcc single crystal copper are performed. Indentation is accommodated by elastic deformation of the surface, up to an indenter displacement of about 4.2 Å, and by nucleation of crystalline defects for deeper indents. The critical load for the event is computed and the nucleation is observed. The result is compared with experimental data. The comparison conveys the conclusion that incipient plasticity is induced at much earlier times and much smaller loads than observed in nanoindentation experiment, and the measured instabilities are collective events involving a large number of pre-existing dislocations.

In load-controlled nanoindentation experiments, after a preliminary elastic stage, a discontinuity in indenter displacement has been captured for the measured load ***P*** versus indentation depth ***h*** response for several crystals. A quantitative understanding of the critical condition for homogeneous dislocation nucleation is still lacking. Experiment and quasicontinuum simulation of nanoindentation in fcc copper are performed. The copper is modeled using the EAM potential [1]. A rigid knife-like flat indenter, 9.31 Å wide, is driven down into the (110) surface of the crystal. Perfect stick conditions between the indenter and crystal are assumed. The model is shown in fig.1. When indented in the [111] direction produces dislocation nucleation from the stress concentration sites at the indenter edge. The critical load for the event is computed and the nucleation is observed. The result is compared with experimental data. The comparison conveys the conclusion that incipient plasticity is induced at much earlier times and much smaller loads than observed in nanoindentation experiment, and the measured instabilities are collective events involving a large number of pre-existing dislocations.

The load versus indentation depth curve for this simulation is plotted in fig. 2. The sudden drop in the load at the instant of dislocation nucleation is clearly visible. The nucleated dislocations are shown by plotting the displacement plots (see fig. 3). Moreover the 22st snap of atoms of nanoindentation by QC simulation is shown (see fig. 4). The dislocations are found.

Figure 1: Nanoindentation model by QC simulation

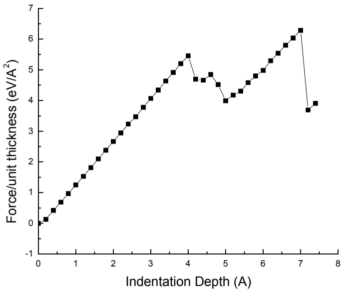

Figure 2: The force per unit thickness versus indentation depth for the nanoindentation simulation

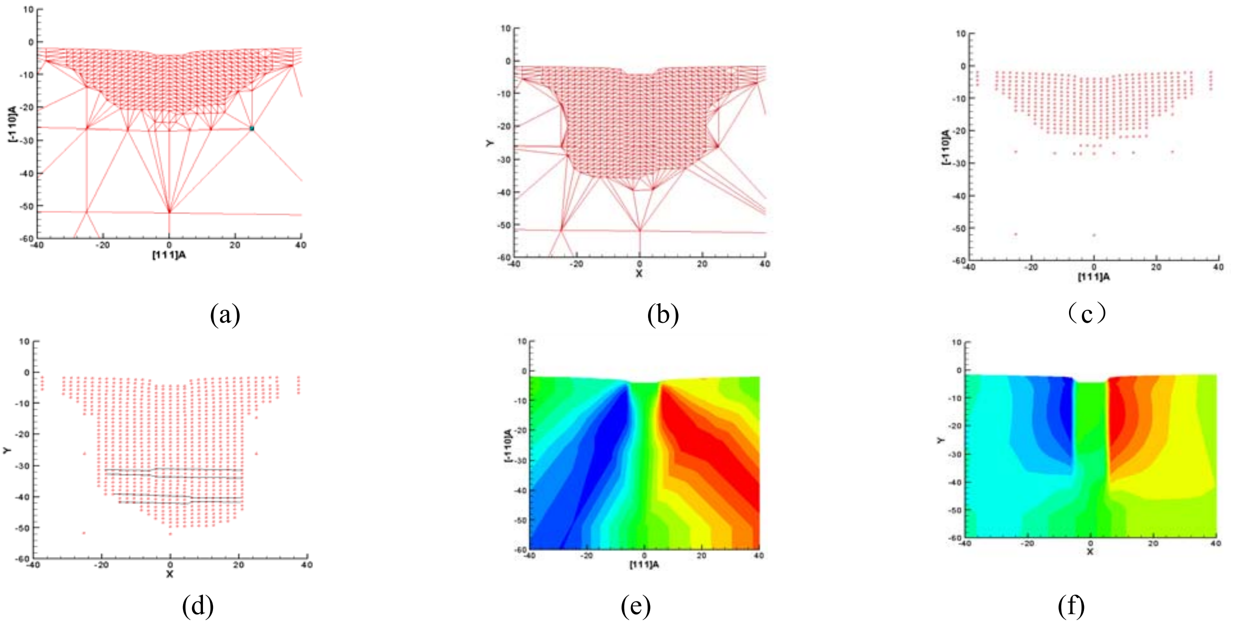

Figure 3: Two snapshots of the mesh under indenter (a) immediately before the first emission, (b) after emission of dissociated dislocations from both ends of the indenter and (c) corresponding snap of atoms at 21st steps (d) corresponding snap of atoms at 22st steps. Frames (e) and (f) show the corresponding scatter plots.

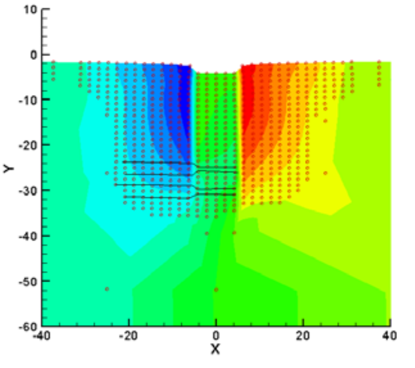

Figure 4: Snap of atoms at 22st steps and contour (UZ)

References:

1. E.B.Tadmor, M. Ortiz, and R. Phillips. Quasicontinuum analysis of defects in solids. Phil. Mag. A, 73(6):1529-1563,1996
2. S.M. Daw and M.I. Baskes. Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. Phys. Rev., B, 33(12):7983-7991