ATOMISTIC SIMULATION OF THE MECHANICAL BEHAVIOUR OF CRACKED NANOWIRES

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The tensile deformation of a cracked cylindrical single crystalline copper nanowire made of 100,000 atoms has been simulated using the *embedded-atom method* [1, 2]. In this method each atom is considered as an "impurity" occupying a site of the lattice formed by the rest of atoms. The atoms experience two types of interactions, as shown in eq. (1): through a *pair potential V*, with the atoms around it, and because of their electrons, through an *embedding potential F* dependent on the relative electronic density ρ, which is calculated with eq. (2).

$$E_i = \frac{1}{2}\sum_{j\neq i} V(r_{ij}) + F(\rho_{ti}) \quad (1)$$

$$\rho_{ti} = \sum_{j\neq i} \rho(r_{ij}) \quad (2)$$

Tabulated data for the embedding and pair potentials for copper are taken from ref. [3]. Forces on each atom are calculated from eq. (1) and their trajectories are calculated by numerical integration of the motion equations [4].

For the present work a cylindrical [001] copper nanowire (fig. 1) of 7.2 nm of diameter and 28.8 nm of length was generated. A transverse crack of circular shape (fig. 2) was introduced on the surface of the nanowire by partial elimination of two (001) atom layers, creating a gap of approx. 0.9 nm. The crack is symmetric with respect to the (010) plane. The net section of the wire has been varied from 2/3 to 1/3 of the total cross section. The two ends of the cylinder remain flat during the test and the atoms there have no restriction in their motion parallel to the end surfaces. The simulations are athermal (0 K) and the tensile tests are performed in a quasi-static way. Starting from an initial equilibrium of the particulate system, axial displacement of the atoms at the end surfaces is imposed at constant steps of 10^{-4} nm. After each displacement step of the boundaries, the force on each atom is derived from the potential and the atoms are moved towards a new equilibrium configuration of the system at very small constant time steps [5].

Figure 3 shows the nominal (remote) tensile stress vs. relative displacement obtained from the calculations for a crack of diameter D_e = 10.8 nm and depth, a, 4.98 nm (see Fig. 2). In this case, the net section at the crack location is only 1/3 of the original one. Figure 4 shows the longitudinal mid-section of this nanowire before the test and Fig. 5 shows three successive stages of the same section after different elongations. The wire remains elastic up to a remote stress of 8.5 GPa, when dislocations start to be emitted from the crack tip, making the crack to advance in a ductile manner. Figure 6 shows the change of the transverse section of the wire through the crack end for the same elongations of Fig. 5. Plastic deformation occurs by alternate activation of {111}<011> systems. Slip steps are evident on the free surfaces.

References

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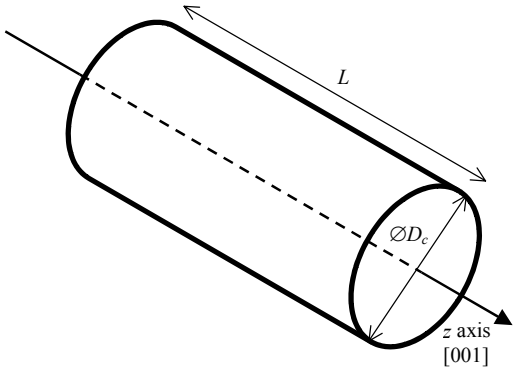


Fig. 1. Geometric characteristics of the tested specimen.

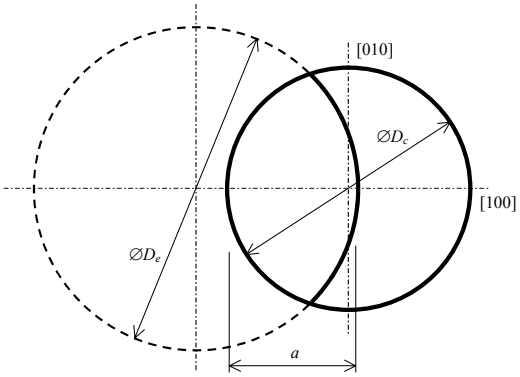


Fig. 2. Geometric characteristics of the crack generated in the surface of the nanowire.

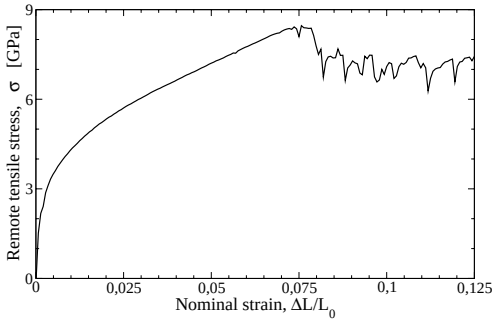


Fig. 3. Nominal stress – strain plot obtained for the simulated sample.

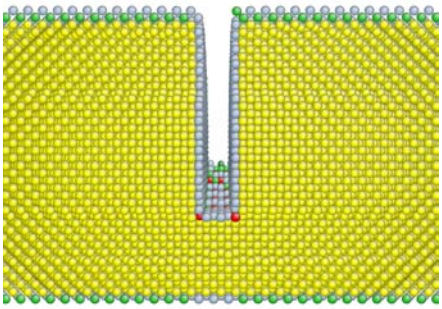
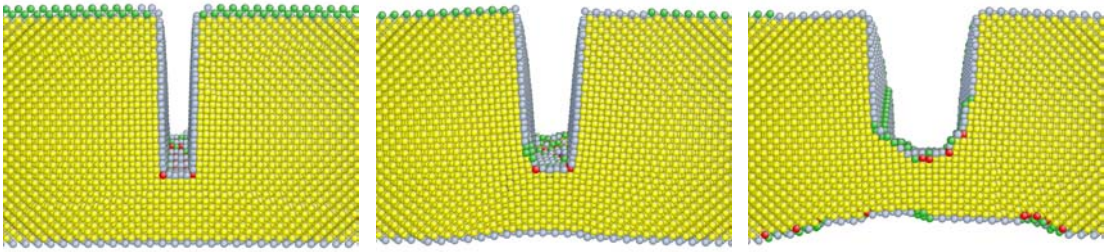
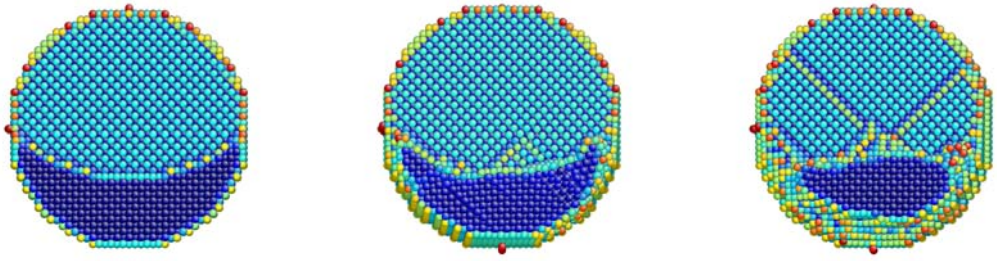


Fig. 4. Initial configuration ($\Delta L/L_0=0$) of the nanowire (colour code according to coordination number [6]). Longitudinal section.



(a) (b) (c)

Fig. 5. Longitudinal sections of the nanowire. The figures show the coordination number of the atoms when (a) $\Delta L/L_0=0.04$, (b) $\Delta L/L_0=0.08$ and (c) $\Delta L/L_0=0.12$. In green, red and yellow, the 10-, 11- and 12-coordinated atoms, respectively. In grey, other coordination numbers [6].



(a) (b) (c)

Fig. 6. Transverse sections of the nanowire across the crack. The figures show the energy of the atoms (using a colour code [6]) when (a) $\Delta L/L_0=0.04$, (b) $\Delta L/L_0=0.08$ and (c) $\Delta L/L_0=0.12$.