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Role of surface on the size-dependent mechanical properties of copper nano-wire under tensile load: A molecular dynamics simulation

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ABSTRACT

In this study we have used atomistic simulations to investigate the role of surface on the size-dependent mechanical properties of nano-wires. In particular, we have performed computational investigation on single crystal face-centered cubic copper nano-wires with diameters ranging from 2 to 20 nm. The wire axis for all the nano-wires are considered along the [0 0 1] direction. Characterization of the initial optimized structures revealed clear differences in interatomic spacing, stress, and potential energy in all the nano-wires. The mechanical properties with respect to wire diameter are evaluated by applying tension along the [0 0 1] direction until yielding. We have discussed the stress–strain relationships, Young's modulus, and the variation in potential energy from surface to the center of the wire for all the cases. Our results indicate that the mechanical response (including yield strain, Young's modulus, and resilience) is directly related to the proportion of surface to bulk type atoms present in each nano-wire. Thus the size-dependent mechanical properties of single crystal copper nano-wire within elastic region are attributed to the surface to volume ratio (surface effect). Using the calculated response, we have formulated a mathematical relationship, which predicts the nonlinear correlation between the mechanical properties and the diameter of the wire.

1. Introduction

Metal nano-wires are essential components in nano electromechanical systems (NEMS) for fast electron conduction. It is established that the conductivity of electrons is associated with the atomic arrangement and defects present within the nano-wires. In addition to conductivity, the structural arrangement also has a considerable influence on the mechanical properties. For example, the diameter of the wire has been shown to influence the yield strength of Nb nano-wires [1] and Au nano-wires [2], and the Young's modulus of Cr nano-wires [3]. Therefore, size-dependent mechanical properties are critical and require further investigation.

Several mechanisms have been proposed to explain the size-dependent mechanical properties. Dimiduk et al. [4] suggested that stochastic effects such as dislocation generation by a stress-dependent source distribution, dislocation trapping, and dislocation escape at free surface would affect the mobile dislocations and source densities and in turn would result in the observed size effect. On the other hand, Greer et al. [5] observed multiple-slip deformation and essentially no work-hardening in their experiments. They suggested that dislocation starvation is the main responsible mechanism. The concept arises due to dimensional constraints that restrain multiplication of dislocations and thus high stresses would be required to nucleate dislocations either in the bulk or from free surface. Volkert and Lilleodden [6] proposed another mechanism based on their observations in which a significant increase in work-hardening is reported with the decrease in pillar size. They explained their observations by a dislocation source-limited mechanism, where the main idea is that the dislocation density is lower in smaller pillars and thus an increase in the applied stress is needed to nucleate or activate new dislocation sources. Since in experiments, even with the state-of-art technology, it is still very difficult to control the defect structure or dislocation distribution in nano-wire or make it defect-free, the observations differ from one study to another and result in different explanations. The most prominent theory describing strengthening with decreasing pillar diameter [7–11] states that the activation of single arm sources is the main mechanism which causes the size-dependent mechanical properties in pillars that range between 200 nm and several microns.

For the very small nano-wires (less than 100 nm), atomistic simulations [12–17] and in-situ TEM analysis [18] demonstrate that dislocations nucleate from free surface. Weinberger et al. [19]

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also used atomistic simulations and transition state theory, as well as continuum modeling, to investigate the dislocation nucleation and strength in gold nano-wire. They concluded that the strength of true metallic nano-wires and nano-pillars (diameters lower than 100 nm) is most likely controlled by dislocation nucleation from free surface. However, the relationship of the size-dependent mechanical response and the atomic arrangement during tensile or compressive load is still not well understood. In particular the mechanical response due to the atoms from the surface to center of the nano-wire is still an open question.

In this study we have used MD simulation to calculate the tensile stress–strain relationship of the entire nano-wire and correlated the mechanical response to the dynamic behavior of atoms in various radial locations during elastic deformation. We have also estimated the effect of size on the mechanical properties of copper nano-wire.

2. Computational method

The nano-wire models in this study comprised of face-centered cubic (FCC) copper, where the wire axes were oriented along the [0 0 1] direction. The diameter of the nano-wires ranged from 2 to 20 nm (2, 2.5, 3, 6, 10, and 20 nm) with lengths of approximately 6 nm. These dimensions were chosen based on the literature [1] which has reported that the mechanical properties are correlated to the reciprocal of diameter. Therefore the surface effects would converge well within the system size range considered and the variation in properties can be reliably related to the characteristics of atoms from the surface to the center of the nano-wire. In order to simulate nano-wires with large length-to-diameter ratios, we set the periodic boundary condition along the axial direction.

In this study we have used a tight-binding (TB) potential [20,21] to simulate copper nano-wires. The TB potential is widely used to predict properties of metals [22–25]. We have adopted the interaction parameters outlined by Qin et al. [26] to describe the copper nano-wire systems. Velocity Verlet integrator [27] with 1 fs time step was used for all the simulations. The Berendsen thermostat [28] was employed to maintain system temperature.

The equilibrium lattice constant of bulk materials was initially used to build nano-wire models; therefore, intrinsic stress exists within the nano-wire. To release this intrinsic stress, simulated annealing and adjustment of axial periodic boundary was employed to equilibrate the atomic structure of nano-wires. The simulated annealing approach used an NVT ensemble to reduce the temperature to near 0 K. During the process, the following convergence conditions between two consecutive steps (10^{-15} s) are implemented: the atomic displacement must be less than 10^{-4} Å, the energy gap must be less than 10^{-5} eV/atom, and the force gap must be less than 10^{-3} eV/Å. These conditions are similar to the conditions used in the high-precision calculation of defects [29]. The adjustment of axial periodic boundary was done by gradually changing length of the axial boundary. The simulated annealing and adjustment of axial periodic boundary were performed iteratively until the residual stress of whole nano-wire is less than ±0.1 GPa.

The structural analysis of the optimized nano-wires were performed with the common neighbor analysis (CNA) [30,31] available within the open visualization tool (OVITO) [32]. For the calculation of stress at the atomic level, the virial stress (local atomic level stress) [33] were used:

$$\sigma_{\mathrm{sys}}^{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N}\sigma_i^{\alpha\beta} \tag{1}$$

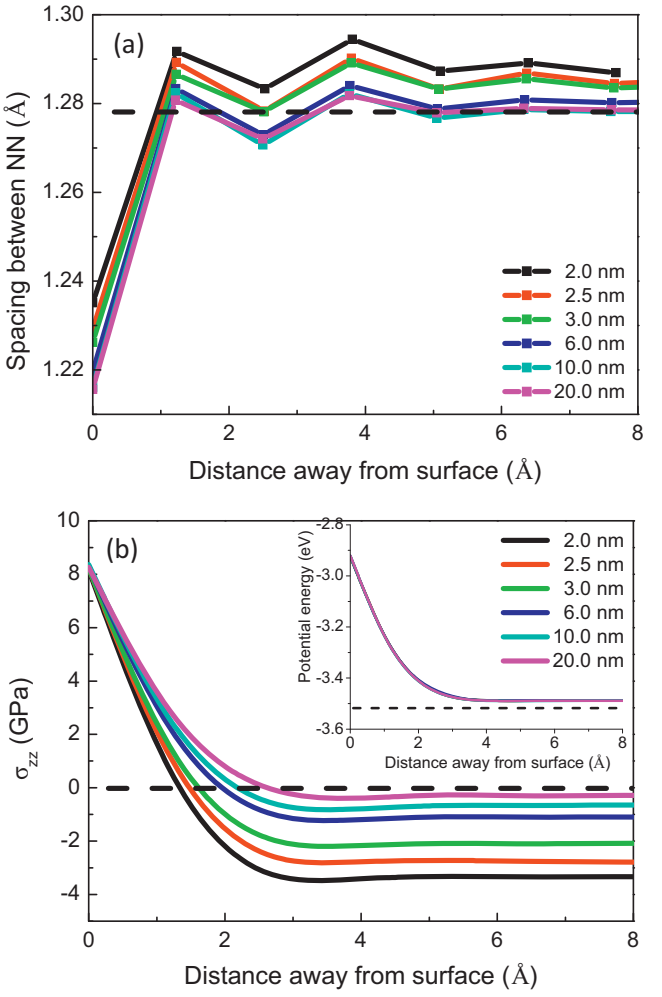

Fig. 1. (a) The spacing between nearest neighboring(NN) atoms and (b) the σ_{zz} of atoms in various radial location along ⟨1 1 0⟩ direction from various nano-wires. The inset in (b) is the potential energy of individual atoms. The black dash lines indicate the corresponding property of bulk copper.

$$\sigma_i^{\alpha\beta} = \frac{1}{2\Omega_i}\sum_{j\neq i} f_{ij}^{\alpha} r_{ij}^{\beta} \tag{2}$$

where $\sigma_{\mathrm{sys}}^{\alpha\beta}$ is the average stress of the system; $\sigma_i^{\alpha\beta}$ denotes the stress on atom i; f_{ij} is the force acting on atom i due to j; r_{ij} is the distance between atoms i and j, and Ω_i is the volume of the hard sphere model of atom i.

The tensile test was achieved by extending the periodic boundary in the axial direction with a strain rate of 4×10^{-7} fs^{-1}, which is equivalent to pulling the nano-wire with a velocity of 2.4 m/s. During the calculations, the system was maintained at near 0 K.

3. Results

Structural characterization of the equilibrated nano-wires shows that atoms toward the center of the wires maintain an FCC arrangement, whereas atoms closer to the surface (top two layers) show significant displacements due to surface optimization and do not maintain the FCC structure. In order to estimate the magnitude of structural optimization, we have quantified the nearest neighbor distance from surface to the center of the wire, i.e. along the [1 1 0] direction for all the nano-wires. Fig. 1(a) presents the change in the nearest neighbor distance calculated for various nano-wires. The results show that the interatomic distance reduces significantly

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