Non linear stress-strain response in ultrathin metallic nanowires. Dependence on the axial orientation.

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Metallic nanowires are a very interesting system from a basic point of view as well as within the context of future nanoelectronics and sensors industry[1]. The mechanical behavior of metallic nanowires under stress has been intensively studied in order to understand their deformation and fracture mechanisms [2-5]. More recently, several studies have focused on the non-linear dependence of stress vs strain in ultra-thin metallic nanowires[6-8]. In this work we examine how non-linear effects depend on the nanowire radius *R*, its cross-section shape and its crystallographic orientation.

We have performed intensive computer simulations to study the stress response (upon both compressive and tensile strain) of Al, Cu and Ni nanowires. The Embedded Atom Method (EAM) potential [9] is used to describe the interatomic interactions. Periodic boundary conditions are used to simulate infinite nanowires. For each nanowire under study we have carried out a Molecular Dynamics (MD) simulation with a stepwise increasing/decreasing strain. At every strain situation we monitor and average the time evolution of the nanowire stress along its axial direction. From the stress vs. strain curve we determine the Young's modulus *E* of the nanowire.

We have considered nine different sets (or families) of fcc nanowires. Each family is characterized by a particular cross sectional shape (rectangular, hexagonal or octagonal) and its main axis orientation (parallel to the [100], [110] or [111] crystallographic direction). Each of these sets contains nanowires of different radii, in order to explore size effects of the mechanical response.

We present results on the distribution of the stress inside the nanowire. These results show that surfaces, and specially edges, accumulate a high tensile stress when compared with bulk regions. Additionally we have observed that nanowires in a relaxed state (stress equal to zero) are slightly shorter along their axial direction compared to the original fcc structure. This contraction of nanowires respect to bulk is stronger for thinner nanowires. Regarding the Young's modulus *E* of nanowires, we have observed the expected trend towards the expected bulk limit value in the corresponding axial orientation when the nanowire cross-section area is larger. However interesting size effects are observed for thinner nanowires. We have observed that the Young's modulus *E* of the nanowires deviates from the corresponding bulk value as thinner nanowires are observed. Whether this deviation is positive or negative is given by the nanowire axial orientation. In this work we explain this size dependence as the result of the non-linear stress-strain behavior of bulk monocrystals, combined with the strong axial contraction that these nanowires experience as thinner nanowires are considered.

The change of the elastic constants when modifying the nanowire radius opens a way to tailor mechanical properties of future nanoscale devices.

References

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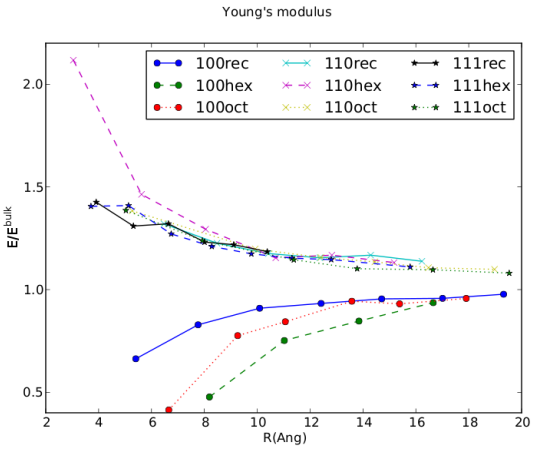
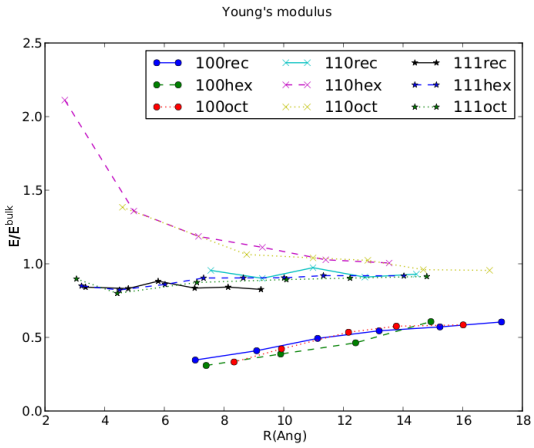
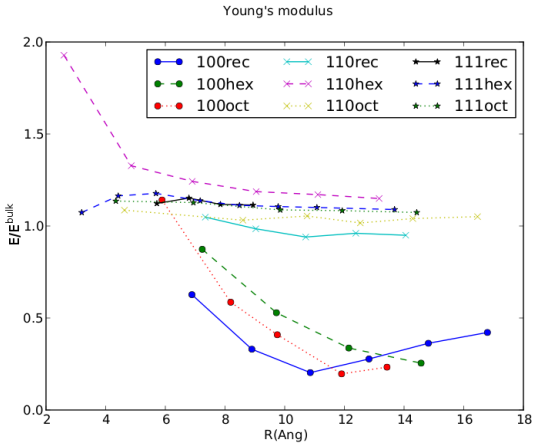
Figures



Aluminum



Copper



Nickel

Young's modulus E of Al, Cu and Ni nanowires as a function of the nanowire radius R. For every nanowire orientation E is plotted in units of E^{bulk} of the corresponding orientation. As R increases, E/ E^{bulk} tends to 1. However, some nanowires orientations exhibit a Young's modulus stronger than the corresponding bulk. The case of Ni along the [100] direction is particularly weird, since the expected trend is not observed.