Size dependence of Young's modulus of metallic nanowires

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Abstract

Metallic nanowires are a system of great technological importance because of their potential applications in nanoscale electronics, photonics, biological and chemical sensors and resonators. A proper understanding of the size dependence of their Young's modulus will lead further in our way to tailor their mechanical properties for practical applications. Although there are several previous studies that deal with the elastic properties of NWs, this issue requires an additional effort in order to systematically describe the dependence of the Young's modulus with NW parameters such as size, external facets, etc.

In this paper Young's moduli *E* of different Al, Cu and Ni ultra-thin infinite nanowires are computed using Molecular Dynamics (MD) simulations, using the Embedded Atom Method (EAM) to describe the inter-atomic interactions [1]. We have considered an extended set of Al, Cu and Ni nanowires configurations to analyze the dependence of the Young's modulus *E* with the nanowire orientation, cross sectional shape and thickness (Figure 1). We also study the character of the stress-strain response in these systems in the elastic phase. Maps of the spatial distribution of the atomic stress inside the nanowire (Figure 2) and its variation with the strain help us to understand the variation of *E* with the different nanowires parameters; also allows us to calculate the "atomic Young's moduli".

Our results demonstrate that the elastic properties of these systems are bulk dominated: Nanowires (NWs) having different cross sectional shapes but the same axial orientation exhibit similar *E* vs thickness trends. respect to the bulk FCC structure.. A non-linear stress response to strain is observed, as reported by other authors [2]. The combination of both this axial contraction and the nonlinear stress/strain observed induces an orientational dependence of the *E* vs *R* curves: As thinner nanowires are studied, the Young's modulus *E* deviates with respect to the bulk value E_{bulk}.

From these simulations we have confirmed and extended previous results by other authors regarding the orientational dependence of the elastic properties in these systems. Nanowire families of different cross-sectional shapes but having the same crystallographic axial orientation exhibit similar trends; in other words, the kind of exposed facets plays a secondary role in comparison with the crystallographic orientation. We have observed a strong nanowire axial contraction of these nanowires with respect to the bulk crystal. This contraction also shows only orientation-dependent trends and compression tends to zero as thicker NWs are considered.

Despite the nanowire orientation, shape or size, the atomic stress of surface atoms is in general positive, the core atoms negative and the difference between surface and core atoms is larger as the nanowire is thinner. On the contrary, the variation of the atomic stress with the strain inside the nanowire depend on the axial orientation (and therefore the "atomic Young's moduli"). For nanowires with [100] orientation, core atoms show a larger variation of stress than the surface atoms when the strain is changed, i.e., core atoms have stronger "atomic Young's moduli" than surface one. For the [110] orientation the situation is reversed, core atoms have a lower "atomic Young's moduli" than the surface. In the [111] orientation we have observed a mixed situation, surface atoms show are 'soft' (low "atomic Young's moduli"), second layer (from surface) atoms are the 'hardest', and core atoms are again 'soft'. As a consequence of these behaviors and because the "atomic Young's moduli" of surface atoms is the dominate term in the thin nanowires (when the number of surface atoms are larger or equal than the number of core atoms), for the [100] nanowires $E<E_{bulk}$, and for [110] and [111] orientations $E>E_{bulk}$,

This work has been partially supported by the Spanish Goverment through projects FIS2012-36113-C01/C02 and CSD2010-00024 (Forces for Future) and by the Madrid Regional Government through the Programs CM-S2009/MAT1467 (NanoObjetos-CM) and CM-S2009/TIC-1476 (Microseres-CM).

References

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Figures

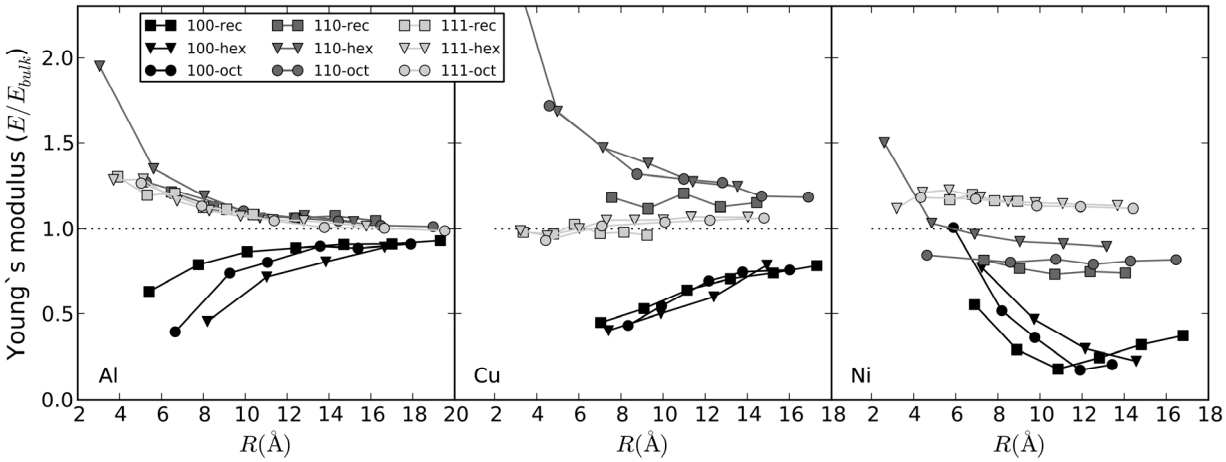

Figure 1: Young's modulus *E* of the nanowires under study. For every nanowire family, *E* is normalized by the bulk value E_{bulk} along the corresponding orientation. The corresponding geometries and crystallographic directions for each curve are indicated in the legend

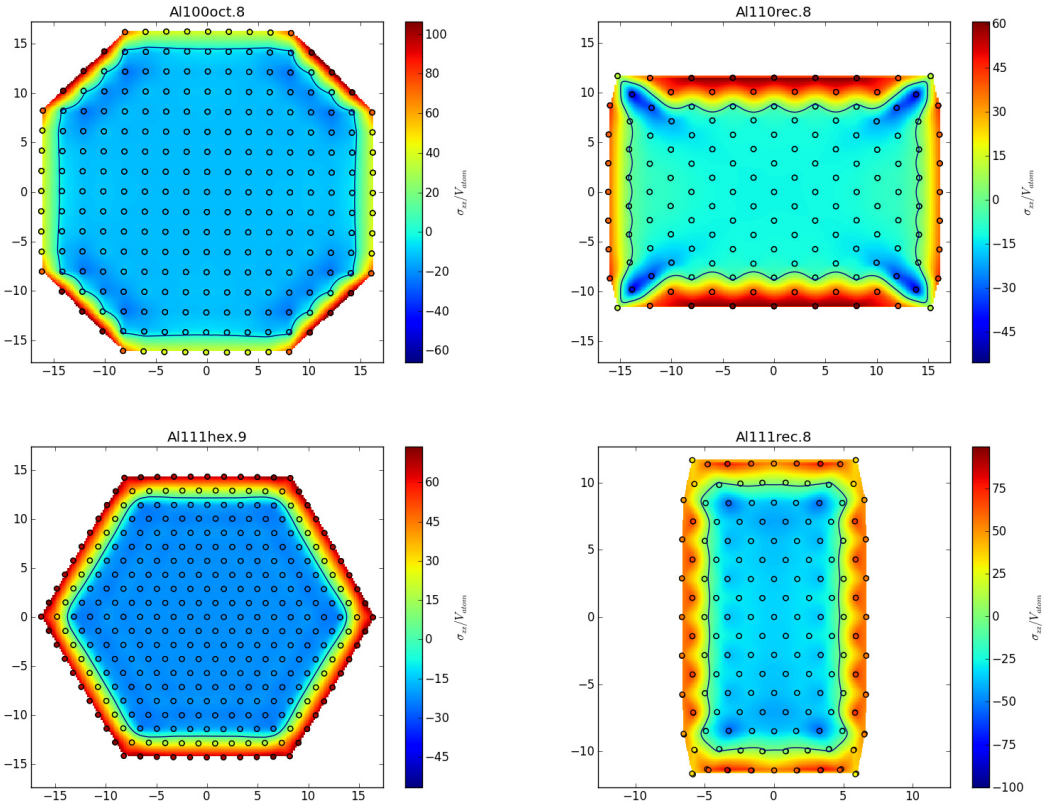

Figure 2: Atomic stress σ_{zz} of the more stable configurations (minimum cohesive energy) for several geometries of Al nanowires. In general surface atoms show a positive stress and core atoms negative stress; how σ_{zz} varies inside the nanowire and with the strain depend on the nanowire geometry