Tailoring mechanical properties at the nanoscale: the dependence of Young's modulus of nanowires on the shape and axial orientation.

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Nanotechnology covers a broad variety of basic and applied studies aiming at the control of different properties at the nanometer level for their use in promising applications. In particular, metallic nanowires are very interesting systems for the basic point of view as well as within the context of future nanoelectronics and sensors industry [1]. The mechanical behaviour 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 focussed on the dependence of the elastic constants on the nanowire size [6], neglecting the role of the orientation and shape of the nanowire. In this work we present the dependence of the Young's modulus of Al and Ni nanowires on three different parameters: cross-section shape and size, as well as the nanowire crystallographic orientation.

We have studied the tensile stress of Al and Ni nanowires by intensive computer simulations. The Embedded Atom Method (EAM) interatomic potential [8,9] is used to describe the energetic of the nanowires. Periodic boundary conditions are used to simulate infinite nanowires. For each nanowire under study we have carried out a conjugate gradients minimization of the cohesive energy in order to obtain its optimal relaxed structure. We have already used this methodology for calculating edge energies [10]. From this equilibrium condition we contract or stretch the nanowire by imposing compressive and tension loads (see Figure 1a and 1b). The nanowire atomic positions are optimized again for the stressed situation, and from these optimized coordinates the local (microscopic) stress as well as the total energy are calculated. From the total energy *versus* strain curve we determine the Young's modulus.

We have considered nine different sets (or families) of crystalline FCC nanowires. Each family is characterised by a particular cross sectional shape (rectangular, hexagonal or octagonal) and its main axis orientation (parallel to the [100], [110] or [111] crystallographic direction). For each family several nanowires of different size (cross sectional area) have been taken into consideration in order to describe size effects.

We present results on the distribution of the stress inside the nanowire. We show that surfaces, and specially edges, accumulate a high tensile stress when compared with bulk regions. Young's modulus tends to the expected bulk limit value in the corresponding direction when the nanowire cross-section area increases. However interesting size effects are observed for thinner nanowires. Young's modulus of [100]-oriented nanowires becomes smaller than the limit bulk value as thinner nanowires are considered (see Figure 2). However, for [110]- and [111]-oriented nanowires the Young's modulus grows for decreasing nanowires diameters. This general trend is slightly dependent on the kind of cross-section shape. This trend agrees with that observed for thin slabs.

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

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FIGURES:

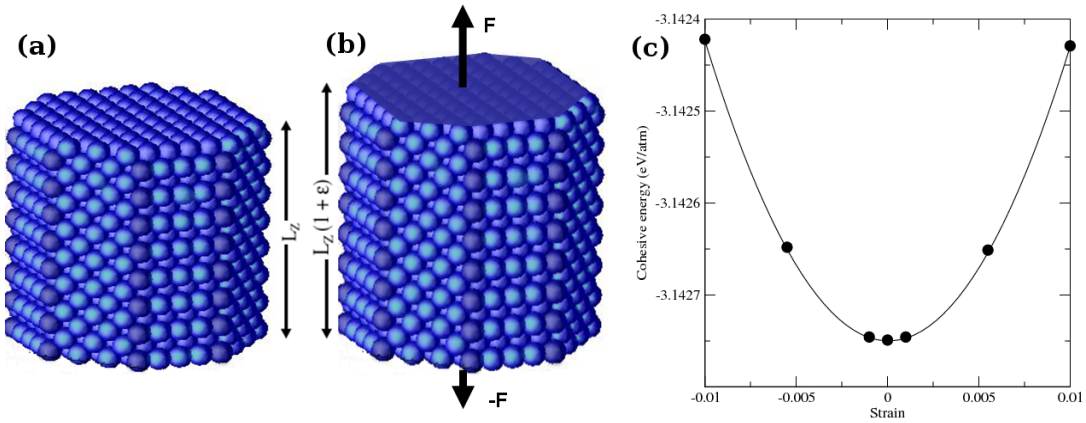

Fig 1. Schematic view of an octogonal nanowire along the [100] crystallographic orientation. Left: original configuration. Right: a strain ε is applied.

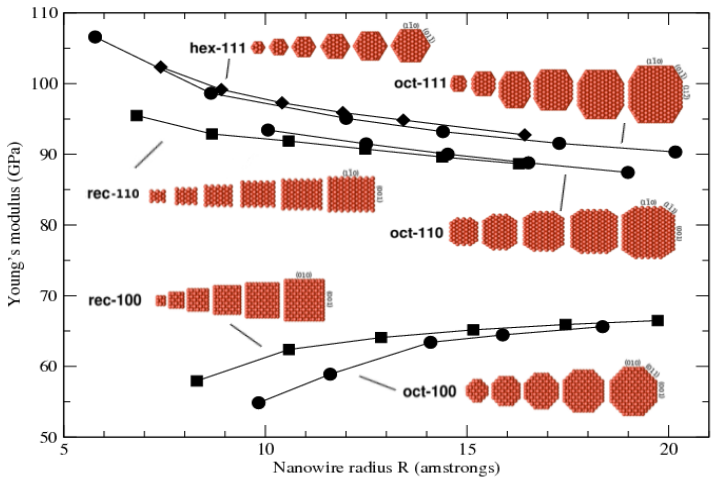

Fig 2. Young's moduli for several families of Al nanowires. Expected