MECHANICAL PROPERTIES OF METALLIC PENTAGONAL NANOWIRES: TEMPERATURE DEPENDENCE

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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 from a basic physics point of view as well as within the context of future nanoelectronics and sensors industry. However, suspended ultra-thin metallic nanowires are rather weak and hardly reproducible structures. Only monatomic chains have been obtained experimentally in a reproducible way, but they are only stable under extremely controlled conditions and at very low temperatures[1].

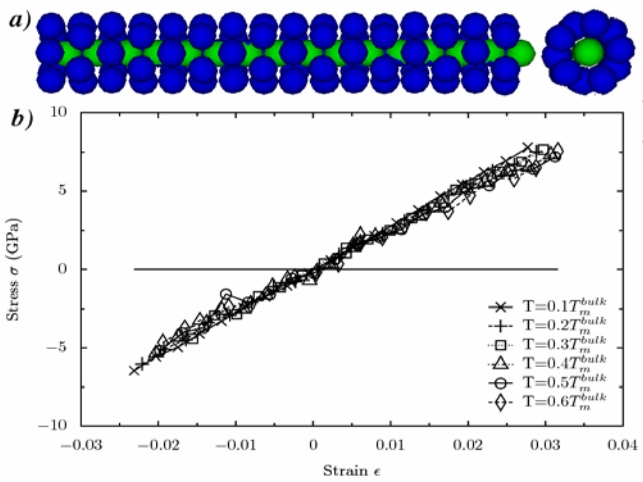
Nevertheless, recent theoretical and experimental studies have pointed towards the possibility of obtaining pentagonal (icosahedral) nanowires consistently from the breaking of metallic nanocontacts in certain conditions [2-5]. These icosahedral or pentagonal nanowires are formed by subsequent staggered parallel pentagonal rings (with a relative rotation of $\pi/5$) connected with single atoms, showing a characteristic -5-1-5-1- ordering (see an example in Fig. 1a). The atomic sequence -1-5-1-5- presents a fivefold symmetry with respect the nanowire axis. This symmetry does not correspond to any crystallographic FCC nor BCC structures. The -1-5-1-5- staggered nanowire configuration may be understood in terms of a sequence of interpenetrated icosahedra. This icosahedral symmetry is very common in very small systems due to the large stability and high coordination characterizing such geometry [6]. Contrary to monatomic chains, icosahedral nanowires are rather robust structures at relatively high temperatures[4] and, therefore, they may be considered as promising candidates for being used as components in nanodevices [5]. For this reason, there is a need to study the mechanical response of these pentagonal nanowires, focussing on its temperature dependence.

In this work we perform Molecular Dynamics (MD) simulations of the elastic properties of Al, Ni and Cu pentagonal nanowires at different temperatures. The Embedded Atom Method (EAM) interatomic potential [7] is used to describe the energetics of the nanowires. Periodic boundary conditions along the nanowire axis are used to simulate infinite nanowires. For each nanowire under study we have carried out a constant temperature MD simulation using a Nose-Hover thermostat. Once thermal and mechanical equilibrium is achieved, the periodic unit cell is strained along the direction of the nanowire axis to simulate the compression or tension of the system. At each strained situation, the system evolves in a NVT ensemble until it reaches equilibrium. Then the virial stress is calculated. At the end of the simulation a stress vs. strain curve is obtained (see Fig 1b), from which the Young's modulus can be extracted. We have considered pentagonal Al, Ni and Cu nanowires formed by 96 atoms (i.e., 16 x -5-1- units). The stress strain curves have all been obtained for temperatures ranging from 0.1 to 0.6 times the bulk melting temperature of the corresponding metallic species.

For all the nanowires and temperatures simulated we show their mechanical response to tension and compression. We present results of the Young's moduli (see Fig 2) and yielding points of these nanowires. We also show that when subject to a low compression, these nanowires prefer to bend forming an 'S' like nanowire, still maintaining their pentagonal structure, instead of collapsing directly into a cluster.

In general we observe that the Young's modulus of these pentagonal nanowires is much higher than that of the bulk metal or other FCC nanowires. This trend has also been observed in previous works [8]. This fact, added to the high temperature stability of these nanowires and the recently proposed possibility of obtaining these nanowires in the laboratory from nanocontact ruptures, opens a window to their potential use in future nanoscale devices.

FIGURES:



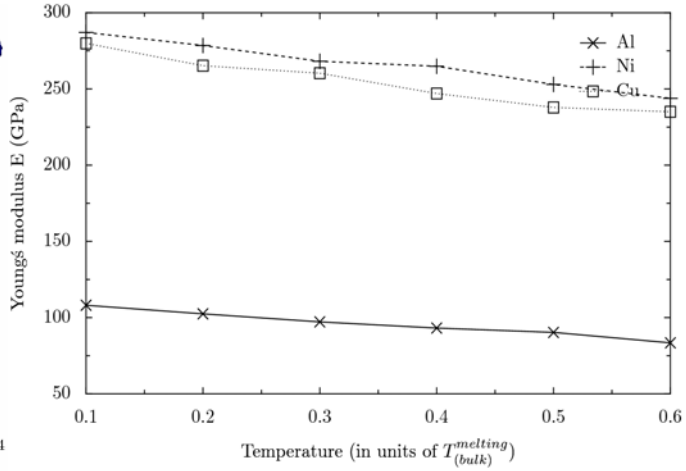


Fig 1: (a) Schematic representation of the pentagonal nanowires under study. Subsequent pentagonal rings are rotated pi/5 and joined by a central (axial) atom. Color (green for axial atoms) is only shown for visualization purposes. (b) Stress vs Strain curves for Cu nanowires at the different temperatures under study.

Fig 2: Temperature dependence of the Young's modulus for the three metallic species under study.

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