COMPUTATIONAL APPROACHES FOR DETERMINATION OF THE MELTING TEMPERATURE OF SUSPENDED METALLIC NANOWIRES.

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During the last two decades, the study of the properties of nanowires has been one of the keystones in the development of nanotechnology, since these nano-objects exhibit electrical and mechanical properties of interest in fundamental knowledge as well as technological applications. In particular, the formation of ultra-thin metallic nanowires from the breaking of nanocontacts has been subject of many experimental and theoretical studies. For instance, the formation of linear atomic chains (LAC) has been observed in both scanning tunneling microscopy (STM) and mechanically controllable break junction (MCBJ) experiments on different metallic species [1]. By means electron beam irradiation of thin Au films long nanowires of helical structures can be obtained [2]. Moreover, theoretical works have shown the formation of a great variety of weird nanowires which present a higher stability than the a priori expected fcc/bcc crystalline nanowires [3].

A few years ago, it has been suggested that icosahedral (a.k.a. pentagonal) nanowires are formed spontaneously in MCBJ ruptures of Cu nanocontacts[4]. In a recent work we have reported Molecular Dynamics (MD) simulations of the breaking process of Al, Ni and Cu nanowires in which these icosahedral nanowires are observed [5]. We have shown that these structures are long, very stable and are formed at relatively high temperatures compared to the corresponding bulk melting temperature. Indeed there is an optimal temperature at which the probability of formation of pentagonal nanowires is highest. The existence of this optimal temperature is the result of a balance between two phenomena. On one hand a high temperature favors the formation of a disordered region in the narrowest section of the nanowire. It is from this disordered region that atoms diffuse to form pentagonal rings. On the other hand, a too high temperature induces the melting of the narrowest section of the nanowire, and the breaking of the contact.

In the present work we are interested in the temperature dependence of the stability of suspended icosahedral nanowires. We use MD simulations to study the dynamical evolution of the nanowires as the temperature increases. In order to have a more consistent methodology different heating rates υ are tested. Infinite pentagonal nanowires are simulated by using periodic boundary conditions along the nanowire axis. Different sizes of the unit cell along the nanowire axis direction are tested, in order to identify size effects in our simulations. Interatomic interactions are modeled using a parameterization of the Embedded Atom Method (EAM). Temperature is controlled by a Nosè-Hover chain algorithm. We have checked that the thermal expansion coefficients in these systems are negligible and were not considered in the simulations.

Here we report the melting temperature T_m of the icosahedral nanowire structures for three metallic species: Al, Ni and Cu. This T_m is determined from a statistical analysis of many MD simulations at different heating rates. For every simulation we monitor the total cohesive energy E_C, Lindemann coefficient, axial component of the stress and angular and radial distribution functions. An abrupt change in these observables indicates that the nanowire has abandoned its pentagonal structure due to thermal diffusion. Massive repetitions of the simulation gives rise to a statistical distribution of temperature values at which this transformation takes place. From this distribution an average melting temperature $<T_m>$ can be obtained. It has been observed that after the pentagonal structure is altered, the nanowire is distorted and becomes a nearly-spherical cluster (see figure 1).

We have observed that the calculated average T_m ($<T_m>$) decreases when the number of atoms N_a used in the simulation unit cell are increased. On the other hand a decrease in $<T_m>$ is observed when lowering the heating rate υ. We expect that the dependence of T_m with both the υ and N_a should converge to a constant value in the limit of slowest υ and largest N_a.

References

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Figures

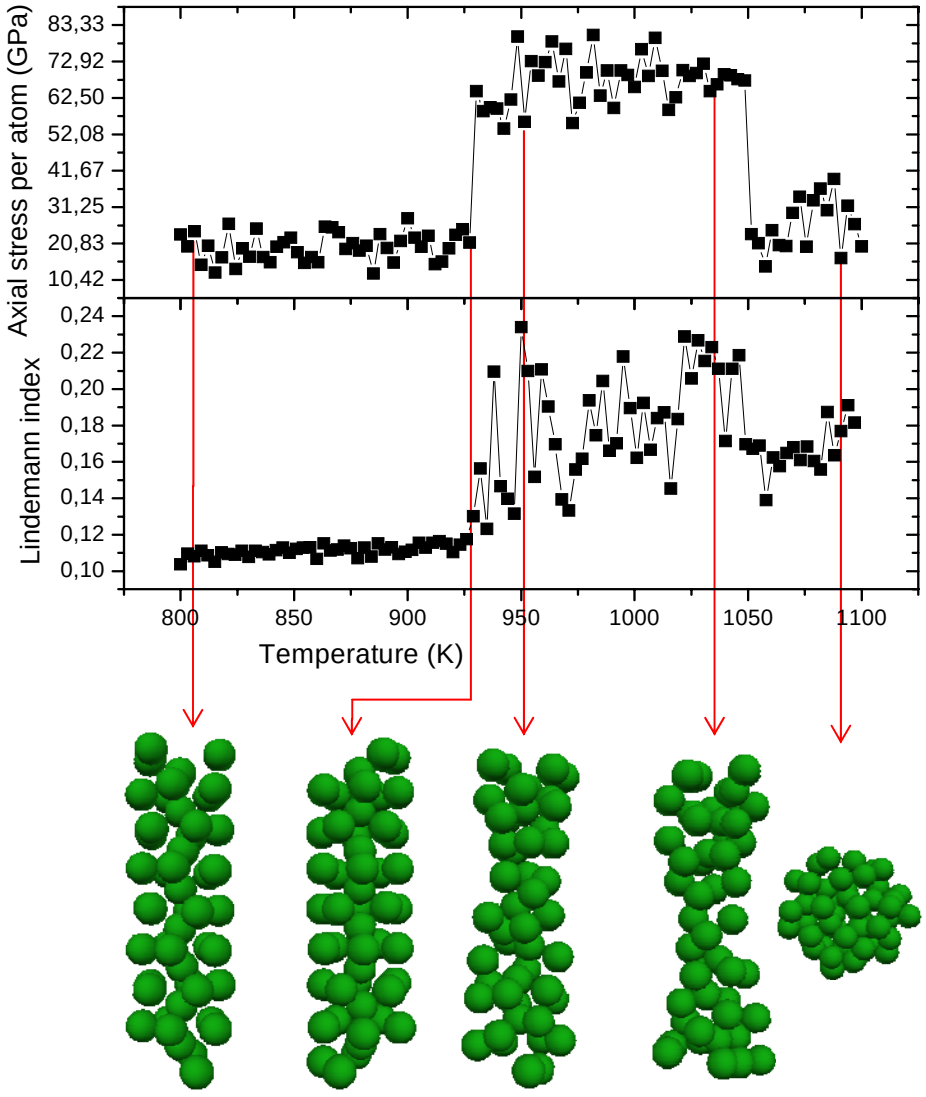

Figure 1. Melting process of a pentagonal nanowire. An abrupt change in both the axial component of the stress or the Lindemann index corresponds to a diffusive distortion of the nanowire's structure. Later, the nanowire breaks and collapses into a cluster.