Melting temperature of icosahedral metallic nanowires

J. A. Pérez Finol (1), S. Peláez (1), P. García-Mochales (2) and P. A. Serena (1).

(1) Consejo Superior de Investigaciones Científicas (CSIC), Instituto de Ciencia de Materiales de Madrid (ICMM), C/Sor Juana Inés de la Cruz 3, 28049-Madrid, Spain

(2) Departamento de Física de la Materia Condensada, C-III, Universidad Autónoma de Madrid, 28049, Madrid, Spain

japerezfinol@icmm.csic.es

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) or 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 the icosahedral nanowires. We use MD simulations to study the dynamical evolution of the nanowires as the temperature increases. 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 taken account the linear thermal expansion coefficients of the pentagonal nanowires.

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 slowly increasing temperature. For every simulation the diffusion coefficient and the total cohesive energy are monitored. An abrupt jump in these observables indicates that the nanowire has abandoned its pentagonal structure. It has been observed that once the pentagonal structure is altered, the nanowire is rapidly distorted and becomes a nearly-spherical cluster (see figure 1). A statistical analysis of the temperatures at which this structural change takes place gives a good estimation of the melting temperature T_m (see figure 2).

References

[1] N. Agraït, A. Levy-Yeyati, and J.M. van Ruitenbeek, Phys. Rep. **377**, 81 (2003).
[2] K. Kondo and K. Takayanagi, Science **289**, 606 (2000).
[3] O. Gülseren, F. Ercolessi and E. Tosatti, Phys. Rev. Lett. **80**, 3775 (1998).
[4] J.C. González, V. Rodrigues, J. Bettini, L. G. C. Rego, A. R. Rocha, P. Z. Coura, S. O. Dantas, F. Sato, D. S. Galvão, D. Ugarte. Phys. Rev. Lett. **93** 126103-1 (2004)
[5] S. Pelaez, C. Guerrero, R. Paredes, P. García-Mochales and P. A. Serena, in preparation**.**

Figures

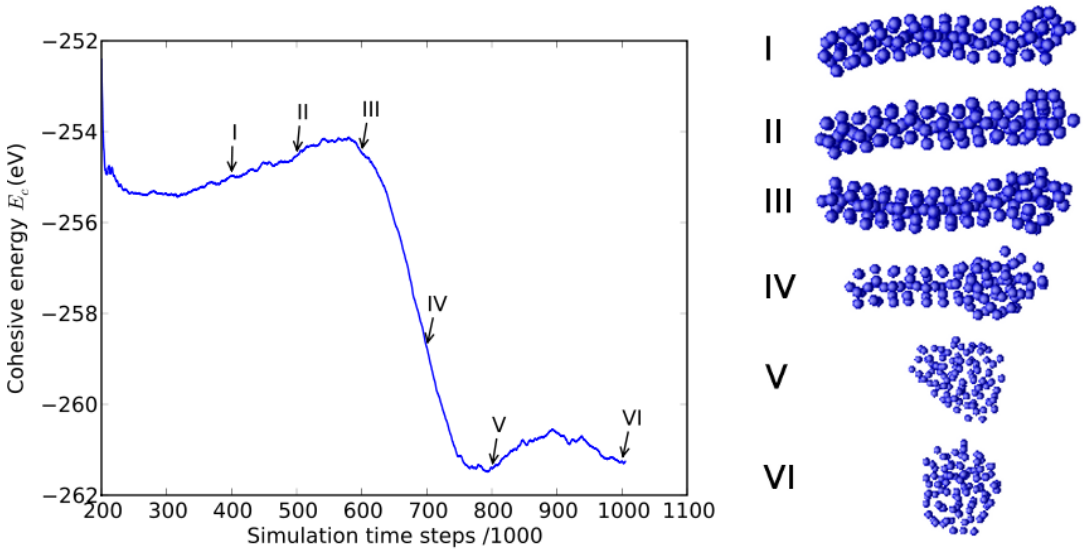

Figure 1. (Right) Time evolution of the cohesive energy E_c during the melting process of a pentagonal Cu nanowire, The cohesive energy E_c exhibits a jump, which clearly indicates that this transformation has taken place. (Left) Several snapshots corresponds to the cu nanowires whose cohesive energy is shown. Note that once the pentagonal structure is distorted due to a high temperature anywhere along the nanowire, it rapidly transform into a cluster.

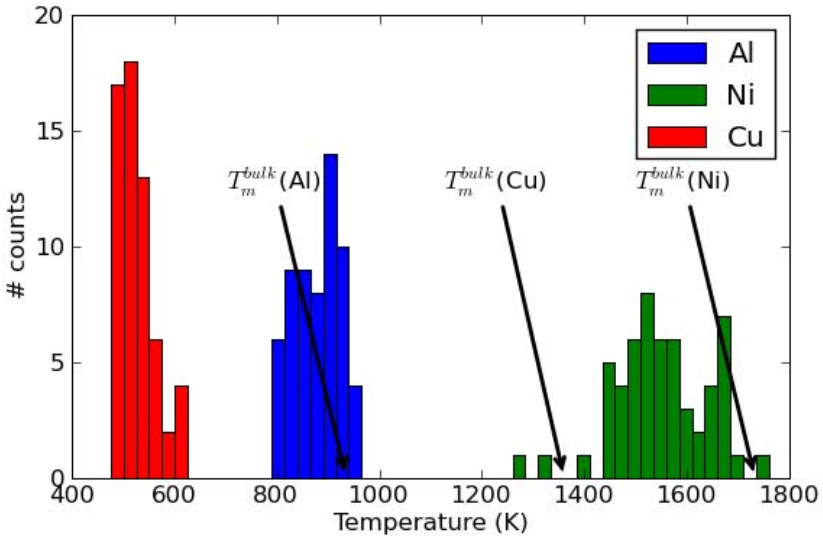

Figure 2. Histograms of the melting temperature of pentagonal nanowires. These histograms have been obtained from 60 independent melting simulations for each material. The arrows point to the melting temperatures of the corresponding bulk system. Notice the large difference between T_m and T_m^{bulk} for the Cu case.