IDENTIFICATION AND CHARACTERIZATION OF ICOSAHEDRAL NANOWIRES ON FCC METALS

S. Peláez[1], C. Guerrero[2], R. Paredes[3], P. A. Serena[1], P. García-Mochales[4,]*

[1] *Inst. de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas (CSIC), c/ Sor Juana Inés de la Cruz 3, Cantoblanco, E-28049-Madrid, Spain*
[2] *Departamento de Física, Facultad Experimental de Ciencias, La Universidad del Zulia (LUZ), Maracaibo, Venezuela*
[3] *Centro de Física, Instituto Venezolano de Investigaciones Científicas (IVIC), Apto. 20632, Caracas 1020A, Venezuela*
[4] *Dept. Física de la Materia Condensada, F. de Ciencias, Universidad Autónoma de Madrid (UAM), c/ Tomas y Valiente 7, Cantoblanco, E-28049-Madrid, Spain*

[*] *pedro.garciamochales@uam.es*

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. 1b). Metallic nanowires are of great technological importance due to their properties and potential applications. Contrary to monoatomic chains, pentagonal nanowires are rather robust structures at relatively high temperatures and, therefore, they may consider as a promising candidate for being used as nanodevice components. Different computational works during the last decade have showed the formation of staggered pentagonal configurations on breaking nanowires of different species [1,2]. 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.

We present a computational method to identify and characterize icosahedral nanowires. This methodology also allows the determination of the pentagonal chain length as well as the number of pentagonal rings that forms it. The algorithm is based in the determination of the angular distribution of the nearest-neighbors atoms and provides a parameter ($\alpha(z)$) which compares the angular distribution of the projected nanowire atomic coordinates with that corresponding to a perfect pentagonal nanowire. This algorithm is applied along the z-coordinate of the nanowire and the result is a $\alpha(z)$ pentagonal profile of the nanowire.

We have tested (Figure 1a) the proposed algorithm for several ad-hoc ordered and disordered structures, proving that it can satisfactorily distinguish staggered pentagonal nanowires from other tubular structures. The initial ordered structures are depicted as inset in Figure 1a, and only in the case of pentagonal nanowire the parameter α takes value 0, being ~1 for the other structures. As the disorder increases, the α average ($\bar{\alpha}$) varies: it increases for pentagonal nanowires and slightly decreases for the other nanowires. If the disorder with respect the initial structure is strong enough, the average of α for all the test nanowires converges to a value ~0.9.

The result of the algorithm applied over a simulated nanowire that presents an icosahedral structure (showed in Figure 1b) are illustrated in Figure 1c: the algorithm returns value near to 1 when is applied to the ordered regions of the nanowire, and values below 1 for the thinnest part of the nanowire. Minima of $\langle\alpha\rangle$ correspond to the position of the pentagonal rings; as they are not perfect ordered structures (but still they can be recognized as pentagons) their $\langle\alpha\rangle$ values are greater than cero. The value $\langle\alpha\rangle$=0.5 discriminates between pentagonal and non-

pentagonal structures. As it can be seen in Figure 1a, non-pentagonal tubular structures (even with strong disorder) have a ‹α› value higher than 0.5. The pentagonal nanowire, even with a relative strong disorder, presents a ‹α› lower than 0.5; a disordered pentagon with ‹α› > 0.5 can not be identified as a regular pentagon. We define the pentagonal nanotube length $L_p(t)$, observed during stretching at a given time t, from the maximum and minimum z coordinates with ‹α›=0.5 as it is shown in Fig. 1c. L_p^m is the maximum value of $L_p(t)$, observed when the nanowire is about to break, and n_p is the number of pentagonal rings forming the icosahedral nanowire at its late stage (equivalent to the number of ‹α› minima below 0.5).

The new methodology has been applied for statistically studying hundreds of breaking nanowire simulations of different metallic species (Al, Cu, Ni) at different temperatures (ranging from 4K to half of its bulk melting temperature), obtaining the maximum pentagonal length L_p^m and number of rings n_p distributions. We have compared these results with the Δt_5 distributions, already used in previous works [2] to identify the existence of pentagonal nanowires (Δt_5 is defined as the time spent by the nanowire with a cross section S_m between 6 and 4 in atomic section units). We show that the quantity Δt_5 generally underestimated the length of the icosahedral nanowire and, as consequence it is not adequate for the characterization of icosahedral nanowires.

References:

[1] R.N. Barnet and U. Landman, Nature 387, 788 (1997); H. Mehrez and S. Ciraci, Phys. Rev. B **56**, 12622 (1997); O. Gülseren *et al.*, Phys. Rev. Lett. **80**, 2775 (1998). J. C. González *el al.*, Phys. Rev. Lett. **92**, 126102 (2004); V.K. Sutrakar and D.R. Mahapatra, J. Phys.: Condens. Matter **20**, 335205 (2008); H. S. Park and J. A. Zimmerman, Scripta Materialia **54**, 1127 (2006); P. Sen *et al.*, Phys. Rev. B **65**, 235433 (2002).

[2] P. García-Mochales, R.Paredes, S. Peláez and P.A. Serena, Nanotechnology **19**, 225704 (2008); Journal of Nanomaterials **2008**, 361464 (2008); Phys. Stat. Sol. (a) **205**, 1317 (2008).

Figures:

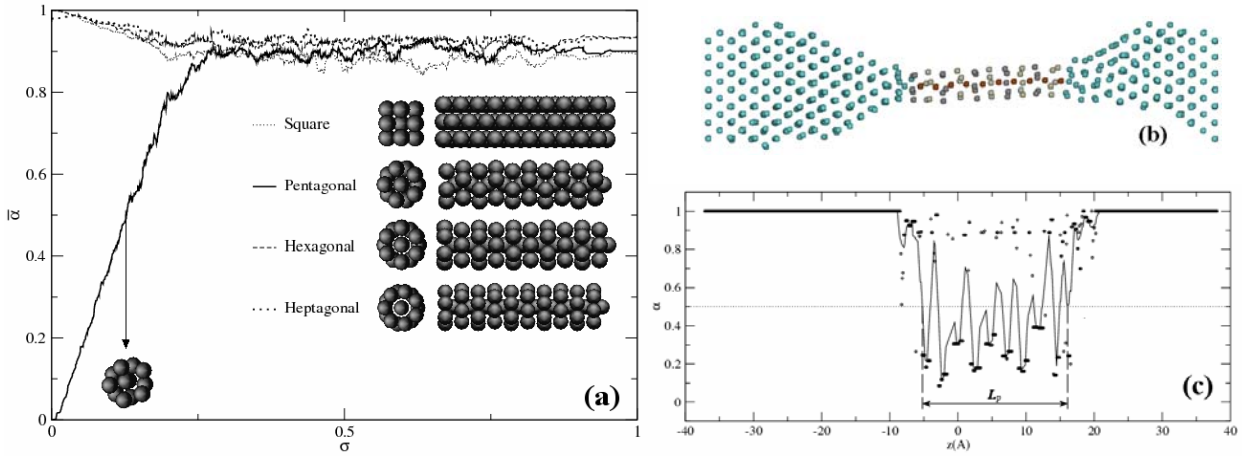

Figure 1 (a) The average of the α-parameter ($\bar{\alpha}$) versus different strengths of the disorder parameter σ for four test configurations: square nanowires with atoms sequence 5-4-5-4 taken from a FCC structure along the [100] direction; staggered pentagonal nanowires with atoms sequence 1-5-1-5; staggered hexagonal 1-6-1-6 nanowires; and staggered heptagonal nanowires with 1-7-1-7 sequence (the inset shows the perfect ordered configurations of the four test nanowires). σ is the mean atomic displacement of atoms with respect to the perfect position of the ordered configuration. The average value of α for disordered nanowires was obtained averaging over 50 configurations. **(b),(c)** Results from Molecular Dynamics simulations of Ni [100] nanowires containing 1029 atoms and subjected to longitudinal stretching at T=375K: **(b)** Snapshot of a nanowire formed under stretching presenting an icosahedral structure with n_p=10 pentagonal rings. **(c)** α-parameter (dots) and its average ‹α› (solid line) along the Ni[100] simulated nanowire of Figure 1b and the icosahedral nanowire length L_p (=21.1 Å). The doted line ‹α›=0.5 is the limit value we have chosen fot the identification of pentagonal structures. The minimum values of ‹α› correspond to the position of pentagonal rings forming the icosahedral nanowire.