CHARACTERIZATION OF ICOSAHEDRAL METALLIC NANOWIRES FORMED UNDER STRETCHING

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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. These structures have been found on simulated nanowires of different species [1-5]. However, the statistical study of their formation has been only addressed for Ni up to date [4,5]. It has been shown that that [100] and [110] stretching direction favour the appearance of long pentagonal nanowires [4,5], and that there exist an optimal temperature at which the pentagonal nanowire yield is maximized [5].

In [4,5] a method based on the time that the breaking nanowire lasts with a cross section S_m~5 (close to that corresponding to a pentagonal ring) was used to detect the formation of -5-1-5- structures. This measure gives a qualitative value of the length of the pentagonal nanowire formed, but not its actual value (deformations of non-pentagonal regions of the simulated nanowire can increase the total nanowire length without an increase the pentagonal zone length). This method can not determinate either the number of pentagonal rings that form the tubular structure. In order to overcome its limitations, in this paper we present an algorithm that allows the automatic identification of pentagonal rings structures as well as the determination of the actual pentagonal nanotube length L_p. With this new tool we have revisited the Ni case, and extended to Al and Cu the statistical analysis of the formation of pentagonal nanowires.

The algorithm is based in the determination of the angular distribution of the nearest-neighbors atoms and provides a parameter α that measures such angular distribution. The average of α ($\langle\alpha\rangle$) over a 1Å thickness slabs differentiates between pentagonal and non-pentagonal structures. If the parameter $\langle\alpha\rangle<0.5$, the set of atoms inside the slab forms a structure similar to that of a pentagonal ring. On the contrary, if $\langle\alpha\rangle>0.5$ the structure presents another structure (bulk like or disordered). Figure 1 (left) illustrates the use of the α-parameter for a nanowire shown pentagonal structures. From this kind of studies we have been able of obtaining the maximum length associated to a given pentagonal wire L_p. By repeating this study for hundreds of nanowire breaking events we have obtained for different conditions (crystalline orientation, initial size and temperature), the distribution of the quantity L_p as well as the probability distribution of the number of pentagonal rings n_p before the nanowire breaking. An example of these distributions is shown in the right panel of Figure 1 (right). This distribution presents a strong dependence on the temperature and the nanowire orientation. In particular we have analysed the optimal conditions for the formation of long pentagonal chains.

The experimental detection of such pentagonal wires is a key point in order to verify the proposed formation of pentagonal nanowires. We propose two different experimental approaches: (i) in STM-like configurations, by measuring changes in peaks heights associated to those conductance values corresponding to the pentagonal structures during the acquisition of conductance histograms; and (ii), in AFM-like configurations, by detecting the force changes associated to the formation of pentagonal rings during nanowire stretching experiments. Figure

2 shows the expected behaviour for the tip-surface force *versus* tip displacement (or time) during the formation of an icosahedral (pentagonal) chain.

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Figures:

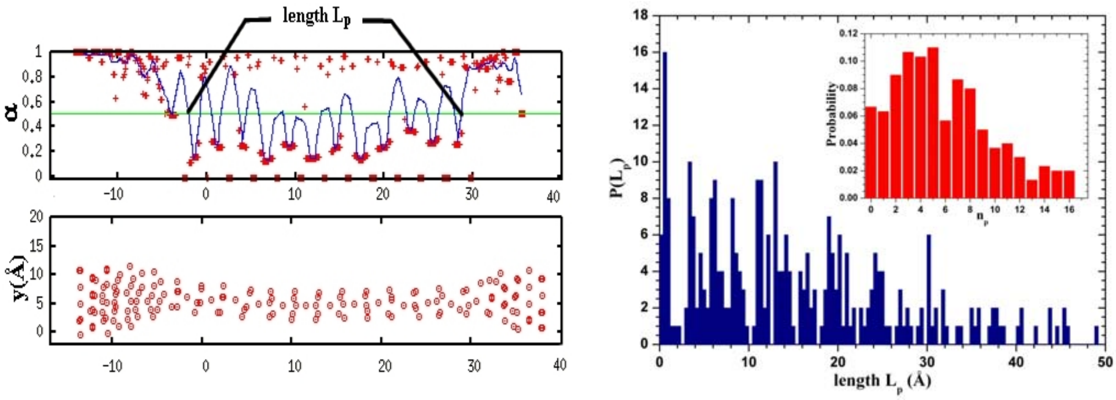

Figure 1: (Left-bottom) yz projection of the atomic coordinates of a simulated Al nanowire with 204 atoms stretched along the [100] direction at 300K. (Left-top) α -parameter (red dots) and its average ‹α› (blue line) along the nanowire. The green line is the reference value ‹α›=0.5. L_p is the pentagonal nanotube length as defined from the maximum and minimum z coordinates satisfying ‹α›=0.5. (Right) Pentagonal tube length distribution $P(L_p)$ and probability distribution of the number of pentagonal rings n_p for nanowires of Al stretched along the [110] direction and 204 atoms at 300K.

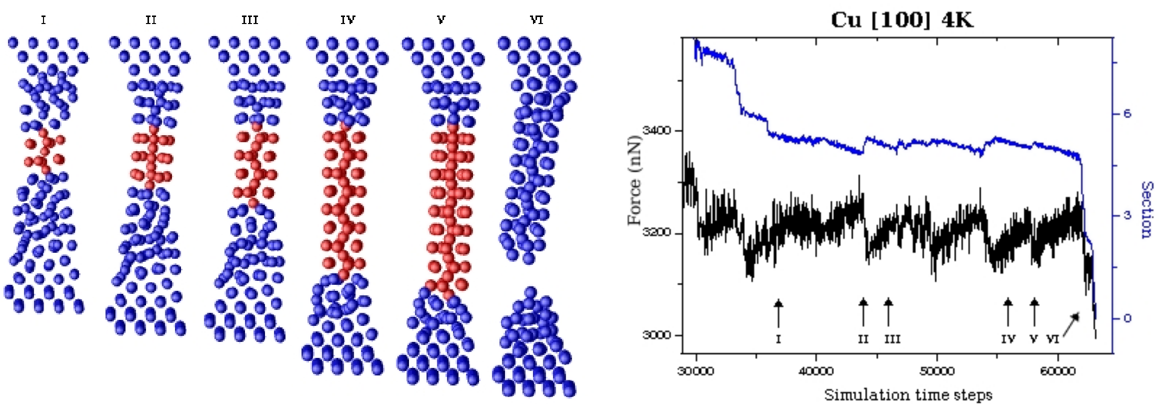

Figure 2 (Left) Snapshots of a Cu nanowire stretched along the [100] direction at T=4K. These images illustrate the formation of an icosahedral or pentagonal chain during stretching (red atoms). (Right) Minimum cross-section evolution (blue line) and force acting on the supporting slabs (black line) upon stretching for the nanowire shown in the left panel. Arrows show the moment at which the left panel configurations have been noticed.