The Discovery of the Smallest Metal Nanotube with a Square Cross-Section

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The study of the mechanical properties of nanostructures presents new theoretical and experimental challenges. The arrangements of atoms in nanostructures and macroscopic matter can be quite different, principally due to the role of surface energy. The interplay between atomic and electronic structure in association with applied mechanical stress can also lead to surprising differences.

Of particular interest are the structures that can not exist at macroscale but that can be stabilized (at least as metastable ones) at nanoscale, especially when stress/strain is present. Examples of these cases are atomic suspended chains and helical nanowires [1].

We present here results showing the spontaneous formation of the smallest possible (one-lattice-parameter-wide) square metal nanotube during silver nanowire stretching [2] (Figure 1). These results were obtained from a suitable combination of time-resolved atomic resolution experiments and ab initio (SIESTA code) theoretical modeling,

The quantum ballistic conductance of these tubular nanowires should be $3.6G_0$ (G_0 conductance quantum). This signature could make the structure possible of identification from electronic transport experiments.

The theoretical analysis suggests that the formation of these hollow structures requires a combination of minimum basis size and high-gradient stress, which could explain why these structures have not been reported before, even from theoretical simulations, where low-stress regimes and small structures have been the usual approach. Our results demonstrate that a proper understanding of the mechanical deformation of nanoscale systems requires the analysis of high-symmetry metastable atomic arrangements. The possibility of the existence of other 'exotic' structures is also addressed.

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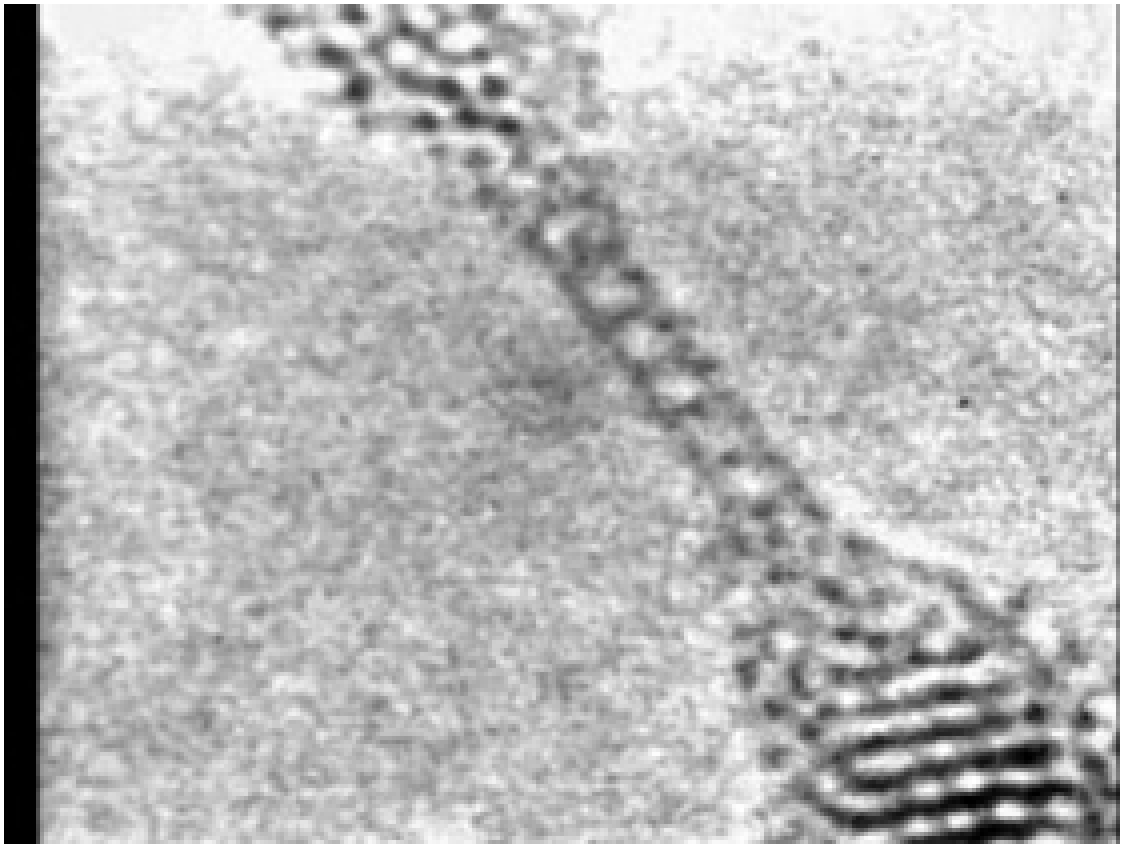
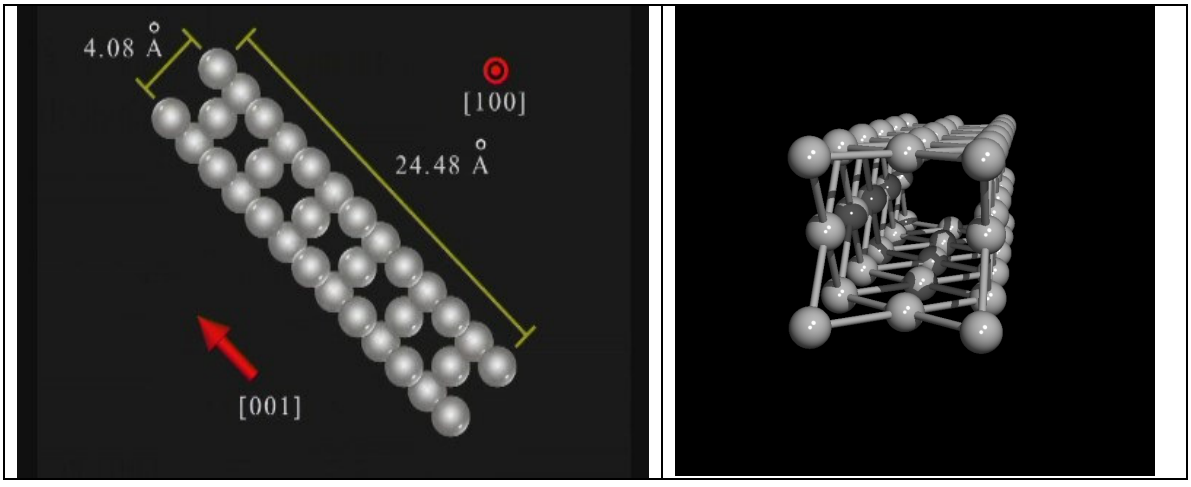
References:

[1] J. Bettini, F. Sato, P. Z. Coura, S. O. Dantas, D. S. Galvao, and D. Ugarte, Nature Nanotechonology 1 (2006) 182.
[2] M. Lagos, F. Sato, J. Bettini, V. Rodrigues, D. S. Galvao, and D. Ugarte, Nature Nanotechonology **4**, (2009) 149.

Figures:



(a)



(b) **(c)**

Figure 1 – (a) High Resolution Transmission Electron Microscopy image showing the observed spontaneous formed square cross section Ag nanotube; (b) Estimated dimensions; (c) frontal view.