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The Smallest Silver Atomic-size Nanotube

M.J.Lagos[(1,2)*], F.Sato [(2)], J.Bettini[(1)], V. Rodrigues[(2)], D.Galvão[(2)] and D.Ugarte [(2)]

(1) Laboratório Nacional de Luz Síncrotron (LNLS), Campinas-Brazil, e-mail: mlagos@lnls.br
(2) Universidade Estadual de Campinas (UNICAMP), Campinas-Brazil
* Corresponding author.

Abstract – We present a study related to the formation and dynamic aspects of the smallest silver nanotube with squared-cross section. Experimental studies were developed by *in situ*-high resolution transmission electron microscopy. Theoretical calculations of total energy showed the nanotube structural stabilization under higher stress conditions. Studies of molecular dynamic allowed analyzing the formation and structural fluctuations of the nanotube during the dynamic process.

The atomic arrangement of nanosystems may be quite different from the traditional materials; surface energy minimization plays a dominant role in this size range, and accounts for many of these new structures. Graphitic nanotubes [1] represent the best example, being fromed by a rolled the graphitic layer, which is traditionally flat. Subsequently the rolling of the compact (111) atomic planes was reported for gold nanowires (NW) generated by mechanical stretching [2]. But, we may expect many more surprises from the interplay between atomic and electronic structure.

Herein, we report the spontaneous formation of a square cross-section hollow metal wires during the elongation of silver nano-contacts along [001] direction. Pure Silver shows a face centered cubic (fcc) metals with almost identical lattice parameter that Au, but subtle changes of the surface energy (cubic facets (100) gain importance) generates clear differences of structural and mechanical behavior as revealed by real time atomic resolution transmission electron microscope (HRTEM).

We have determined the structure of the silver nanotube (Figure 1) by associating time-resolved atomic resolution HRTEM, and also image simulations [3]. Our results revealed that: (i) the hollow NW atomic structure is formed by 2 different atomic planes (A,B), each one containing four atoms, keeping the stacking sequence $4_A/4_B$, instead of the $5_A/4_B$ stacking present in the perfect fcc [001] wire (Figure 2). The total energy theoretical calculations (DFT- *ab initio*) show that this anomalous structure can be stable under higher applied stress conditions.

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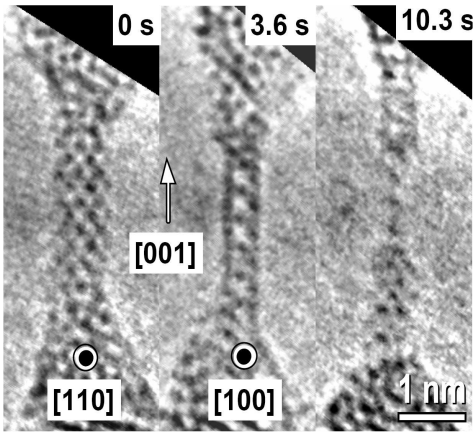

Figure 1: Thinning of a Ag NW being elongated along the [001] axis. Note that significant changes of the NW image (from 0 to 3.6 s) occurs during elongation; finally the wire forms an atom chain (10.3 s) before breaking (atomic positions appear dark).

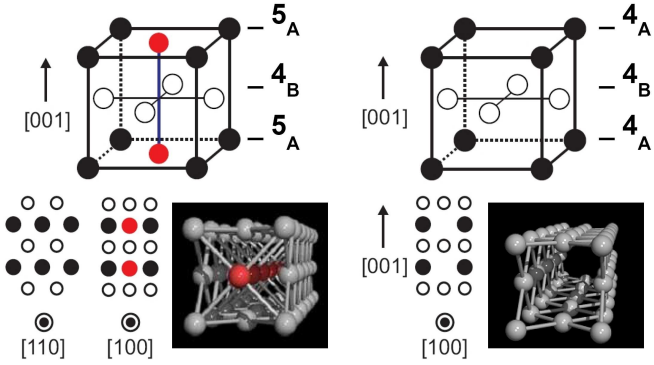

Figure 2: Left: Schematic drawing of a fcc unit cell, and the expected image contrast when a [100] wire of width *a* is projected along [110] and [100] directions; Right: fcc unit cell and expected contrast patter along [100] direction after eliminating the atom located at center at the cube [001] facet), what generates a one-lattice wide Ag hollow NW

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