INTERPRETATION OF THE APERIODIC HRTEM CONTRAST OBSERVED IN GIANT ICOSAHEDRAL GOLD NANOPARTICLES

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It is well known that the shape of gold particles of few nanometers show morphologies which includes cubo-octahedral, octahedral, truncated octahedral, icosahedral, pentagonal decahedral shapes and their twinned variants [1, 2]. In fact, the structural size evolution has been described from specific “molecular” structures, with diameters around 1nm and following the “magic numbers”, to ordered decahedral structures with diameters bigger than 2nm, and reaching the fcc structure and faceted morphologies [2, 3]. In a recently previous work we presented the evidence of the existence of rounded gold nanoparticles with a “quasicrystalline” contrast that resembles that one of the five-fold symmetry contrast of the icosahedral quasicrystalline phase [4]. These nanoparticles have a size diameter of 15 nm approximately, and their high-resolution electron microscopy (HRTEM) contrast could be interpreted in basis of a Moiré contrast produced in Mackay icosahedral particles. In this work we have carried out the structure analysis of their HRTEM image contrast using a simulated Mackay gold icosahedral particle through HRTEM image simulation. This has indicated us that their contrast can be interpreted in basis of the structure of Mackay icosahedra.

Stable gold nanoparticles were prepared by the Brust method [5]. Special interest was done in the contrast presented by giant icosahedral particles along the five-fold axis (fig. 1). HRTEM images and electron nano-diffraction was conducted in a FEI-Tecnai G2 F20 X-Twin microscope operating at 200 kV. For simulation an icosahedral particle of 9.2 nm in diameter was grown. With the files of the (x, y, z) coordinates of the atomic sites of the generated icosahedron, simulated HRTEM images, tilting and diffraction patterns were obtained with the SIMULATEM software. Once obtained the simulated images, an amorphous carbon substrate was added to each one using the SIMULATEM, Digital Micrograph (GATAN) and Photoshop programs.

Simulation and analysis of the contrast experimentally observed in icosahedral gold nanoparticles of 15 nm in diameter along the five-fold direction is presented in this work. The contrast shows, besides a central defect consisting of a line crossing the particle along its diameter, ten-spots rosettes and pentagonal motifs that resembles the contrasts observed in quasicrystalline structures. A detailed analysis demonstrates that these particles are Mackay icosahedral particles slightly tilted from the five-fold axis and that a Moiré-pattern artifact produces the quasicrystalline arrangement observed.

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Figure 1. Comparison of the experimental (at the right) and simulated images (in the inset). For simulation a Mackay gold icosahedral particle of 9.2 nm in diameter was used. It was tilted by $2^\circ$ and the amorphous carbon substrate was included. Note the straightforward similitude.

References