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High Index Faceting in Gold Decahedra Nanoparticles

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Five-fold nanoparticles have been the subject of many scientific studies for over 40 years due to the forbidden five-fold symmetry and because of the potential applications in catalysis [1]. If we take five FCC tetrahedra and put them together a gap of 7.35^o remains between two (111) faces. This gap has to be closed somehow by straining the crystal structure of the tetrahedral sub-units. It has been shown [2] that in fact tetrahedral nanoparticles have a strained lattice that compensates the gap and stabilizes the particle. However, recent calculations show that the highest concentration of strain is located at the surfaces.

In the present work we analyze by aberration-corrected Scanning Transmission Electron Microscopy (STEM) the surface steps of 300 nm Au decahedra. The analyzed decahedra nanoparticles present undulations at the (100) surfaces indicating the presence of high index crystal planes, which seems to be yet another mechanism to release strain. Also, reentrant surfaces are observed at the end of each twin plane, interestingly these surfaces are somewhat asymmetric in some twin planes that may be due to the fact that not all the twin planes are subject to the same amount of strain. Weak beam dark field (WBDF) was also employed to analyze the strain field on decahedra nanoparticles. However, smaller decahedra nanoparticles, around 90 nm, were used for this since big nanoparticles present a poor contrast. The contour fringes appear much distorted confirming the nanoparticle is under strain, also, the intensity of the fringes varies from the center of the decahedron to the surface, being the last fringe at the surface brighter than the other ones. This confirms that the surface holds much of the strain in the particle.

Gold nanoparticles were synthesize by stirring 5 ml of ethylene-glycol (EG) with a magnetic bar and heat up to 250^o C for 10 min. Then, two solutions were prepared separately. For the first one 0.208 g of Polyvinylpyrrolidone (PVP) dissolved in 5 ml of EG. The second one 0.08 g of HAuCl4 were dissolved in 5 ml of EG. Both solutions were injected simultaneously drop by drop in a hot solution of EG. The reaction was carried around 10 min until the solution became orange-purple, indicating the formation of gold nanoparticles. The products were collected by centrifugation at 4,000 rpm for 4 min and washed with ethanol several times. Finally the solution was drop-casted on a copper grid for TEM characterization.[3]

References

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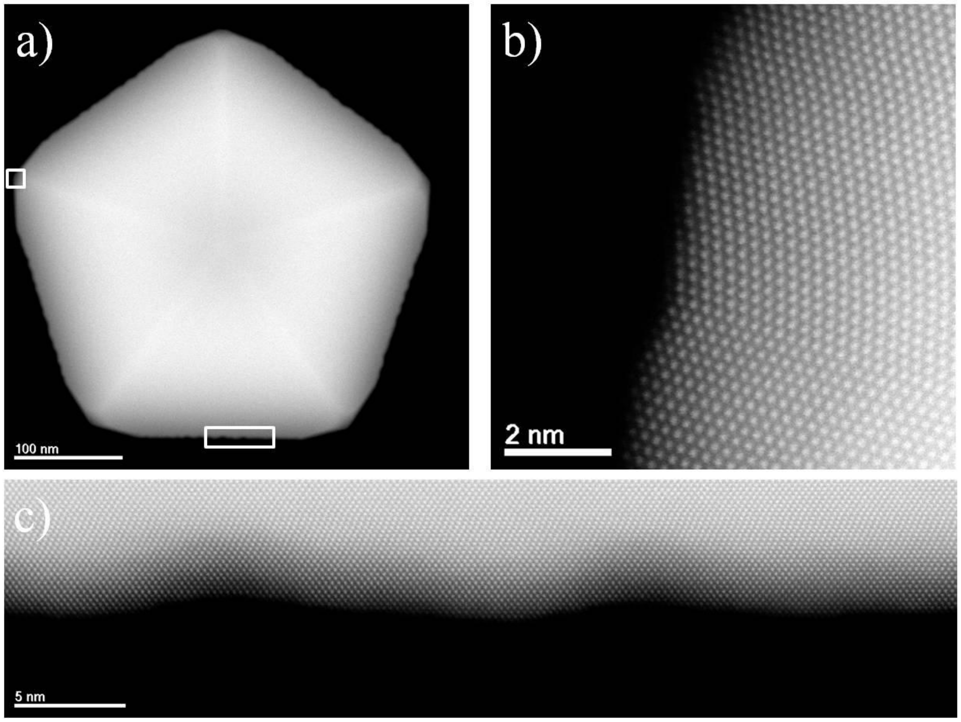

FIG. 1. a) High angle annular dark field image of an Au decahedra in its five-fold axis. It is evident that the surfaces present some undulations. b) High resolution image of the tip marked by the square in a) showing the reentrant surfaces at the twin boundary. c) High resolution of the area marked by the rectangle revealing the high index planes faceting of the decahedra.

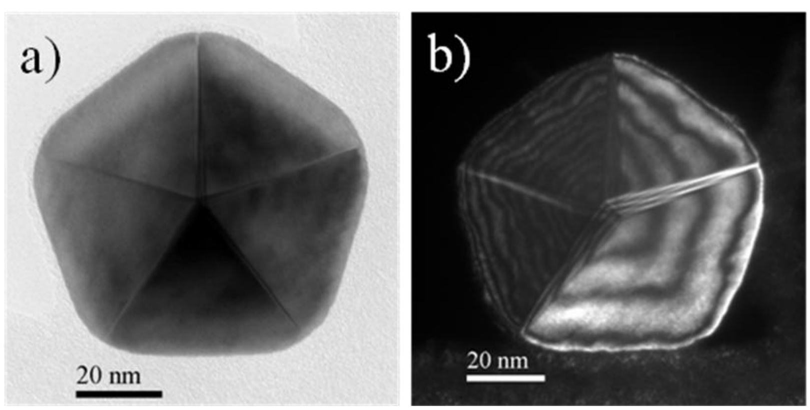

FIG. 2. a) Bright field image of an Au decahedron in the <110> zone axis. b) WBDF of a) showing bent contour fringes. The more intense fringes are clearly on the surface indicating a high strain concentration.