

## Surface stress effects in gold nanocrystals

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Gold is a noble metal towards almost all environmental species with the exception of sulphhydryl-containing species, such as thiols, which readily form monolayer coatings of high stability. The structure of the sulphur-gold interface is remarkably complex. A recent crystallographic study of a monodispersed Au<sub>101</sub>RS<sub>44</sub> gold nanoparticle-thiol complex revealed a crystalline core particle coated with a shell of 1nm thickness with enlarged Au-Au spacings and interpenetration of the thiol ligand species. Far from having a well-defined boundary between the metal and the organic sides of the interface, this unusual complex was found to contain a mixed compound layer as its lowest energy configuration [1]. In this talk I will present the structure of faceted gold nanocrystals before and after coating with propane thiol, one of the simplest SAM-forming organic molecules. The structure of a single 300nm-diameter particle was measured using the powerful technique of Coherent X-ray Diffraction (CXD), which is highly sensitive to the pattern of internal strains within the nanocrystal [2]. The results show that the strain is modified by the thiol adsorption. We have used finite element calculations to establish the magnitude of this stress difference and find it to be quite large.

[1] "Structure of a thiol monolayer-protected gold nanoparticle at 1.1 angstrom resolution" P. D. Jadzinsky, G. Calero, C. J. Ackerson, D. A. Bushnell and R. D. Kornberg, *Science* 318 430-3 (2007)

[2] "Coherent Diffraction Imaging of Strains on the Nanoscale", I. K. Robinson and R. Harder, *Nature Materials* 8 291-298 (2009)

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