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**Pair Distribution Function Analysis Applied to Multiply-Twinned Gold Nanoparticles** CORINNE SILKWOOD, HEINZ NAKOTTE, EDWIN FOHTUNG, New Mexico State University, KATHARINE PAGE, HSUI-WEN WANG, GRAHAM KING, Los Alamos National Laboratory — Pair distribution function (PDF) analysis is a statistically based method of structure determination which investigates the correlation of atomic positions within a sample. Motivated by electron microscope images of gold nanoparticles with non-crystallographic morphologies and the possibility of studying their structure with PDF analysis, three computer models were created. The particles exhibit five-fold symmetry inconsistent with a continuous crystal lattice and generally explained by multiple twinning of a tetrahedral subunit about a symmetry axis, with or without structural modification to the crystal lattice. In cubic structures, five-fold twinning results in a particle with a solid gap; small lattice deformations produce a spatially continuous particle with orthorhombic structure. These alternative geometries, and a hybrid configuration, were modeled. PDF data was simulated for the model particles with the objective of determining sensitivity to twinning and lattice distortion. The simulated data reflects structural characteristics of the models including deformations of lattice parameters on the order of tenths of Angstroms. Subsequent experimental PDF analysis of these particles showed agreement with a twinned cubic lattice model.

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