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Local Structure of Decahedral Gold Nanoparticles

HEINZ NAKOTTE, New Mexico State University, Las Cruces NM

The five-fold symmetry FCC-derived nanoparticles is inconsistent with the translational symmetry of a Bravais lattice and it is generally explained by multiple twinning of a tetrahedral subunit about a (joint) symmetry axis, with or without structural modification to the *fcc* motif. In order to verify theoretical models, it is therefore pertinent that the local structural features of such materials can be fully characterized. The small size of nanoparticles severely limits the application of traditional analysis technique, such as Bragg diffraction. We present the application of Debye scattering and Pair Distribution Function (PDF) analysis towards modeling of the total scattering data for the example of decahedral gold nanoparticles. PDF measurements provide a statistical description of the pair correlations of atoms within a material. We explored the sensitivity of existing neutron and synchrotron X-ray PDF instruments using different models for decahedral gold nanoparticles: a multiply-twinned FCC decahedron model with a gap, a relaxed body-centered orthorhombic BCO and a hybrid model. The predictions of the three models were then compared with experimental data from synchrotron X-rays and we present our experimentally derived atomistic models of the gold nanoparticles, with surprising results and a perspective on remaining challenges. Our findings provide evidence for the suitability of PDF analysis in the characterization of other nanosized particles that may have commercial applications.