

W0101

Pair Distribution Function Analysis of Nanosystems. Katharine Page, Ram Seshadri, Anthony K. Cheetham, Materials Research Laboratory and Materials Dept., Univ. of California, Santa Barbara, CA.

The limited translational periodicity in nanomaterials renders reciprocal space methods of limited utility for structural studies, but real-space methods are showing a great deal of promise. Our early work with 5nm gold nanoparticles demonstrated the power that pair distribution function refinement can bring to structural descriptions on the nano-scale.¹ These results will be presented, along with our more recent study of gold nanoparticles under pressure. We shall also describe the use of total neutron scattering powder diffraction patterns and the pair distribution function to attain quantitative structural information for other nanoparticle systems, including core-shell hard-soft magnetic metal oxides and novel intermetallics. We will demonstrate the problems arising from incoherent hydrogen scattering that are inherent to organically capped nanoparticles, and present complementary synchrotron x-ray data for some of our systems. The potential applications, power and current limitations of real-space methods for analysis of structure in the nano-regime will be discussed.

¹K. Page, Th. Proffen, H. Terrones, M. Terrones, L. Lee, Y. Yang, S. Stemmer, R. Seshadri, A. K. Cheetham, Direct observation of the structure of gold nanoparticles by total scattering powder neutron diffraction, *Chem. Phys. Lett.* **393** (2004) 285-288.