

Poster Presentation

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Size-dependent non-space filling atomic packing in metallic nanoparticles

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Ni-Pd nanoparticles synthesized for CO catalysis are characterized by transmission electron microscopy and total X-ray scattering. The sizes of these nanoparticles can be tuned to size with great control over the monodispersity of the samples. The pair distribution functions of the reveal a local ordering within the highly disordered atomic structure within the nanoparticles. The PDFs show a size-dependent deviation from typical bulk face centered cubic (fcc) structure for these materials. The long-range isotropic disorder within these non-fcc nanoparticles can be fitted using an exponentially damped single-mode sine wave. Below a diameter of 5 nm, the Ni-Pd nanoparticles exhibit local ordering of atoms as found in typical icosahedral clusters. The transition from fcc to non-space filling atomic packing of icosahedral clusters in a nanoparticle is modeled to show the structural origin of the observed PDFs. Understanding this type of disorder can give insight into structure-property relations for applications in heterogeneous catalysis.

Keywords: total X-ray scattering, pair distribution functions, nanoparticles