Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Ab initio modeling of EXAFS spectra of nanoparticles

SAMUEL CHILL, The University of Texas, AARON YEVIK, ANATOLY FRENKEL, Yeshiva University, GRAEME HENKELMAN, The University of Texas — The structure of nanoparticles in the 1-3 nm range is often investigated using extended x-ray adsorption fine structure (EXAFS). Structural information for nanoparticles is typically determined from the fits to EXAFS data using the bulk structure for theoretical calculations. The average coordination numbers, interatomic distances, and their mean squared disorder can be found. The applicability of this procedure is less obvious when the particles are strongly disordered, i.e., when there are significant structural differences between the nanoparticles and the corresponding bulk structure. We use molecular dynamics (MD) simulations of 2 nm nanoparticles to construct EXAFS spectra ab initio, with the atom-by-atom approach, averaged over the time of the MD run. We obtain that the analysis of this data done by conventional procedures reveals significant differences between the actual (time- and configuration- average) structure of the simulated nanoparticles and what was determined from data analysis using a bulk reference. We demonstrate that EXAFS spectra calculated for a variety of theoretical models of nanoparticles can be directly compared to the experiment and thus used to determine the best-fit structure.

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Date submitted: 11 Nov 2011 Electronic form version 1.4