



17th May 2011 - 11:00 am
DESY Building 49 - Seminar Room (108)

Kenneth Beyerlein

Georgia Institute of Technology
GRA Material Science & Engineering Department

Characterizing nanoparticles with Debye function analysis and atomistic simulation

Detailed statistical characterization of nanoparticles is becoming more important as their potential industrial use increases through applications like catalysis, biosensors and drug delivery. Diffraction offers a promising, widely available technique which contains average structural information over many length scales. In wide-angle powder diffraction this information is contained in the broadening and shape of the line profiles. Study of the peak profiles allows for determination of not only particle size, but also particle shape and defect densities. The presented research focuses on a modern line profile analysis approach called Debye function analysis, which simulates the powder diffraction pattern from atomistic models. As case study, the characterization of a wet chemically synthesized Pt nanoparticle sample will be discussed to demonstrate its capabilities.

The Debye function also offers an exciting bridge between atomistic simulations, like molecular dynamics, and experiment. This allows for a controllable study of how microstructure features, and dynamics affect the diffraction pattern. As an example, the lattice dynamics of two fcc metals at a range of temperatures will be presented to study the Debye-Waller temperature factor. In the coming years this combined effort is sure to extend the theory surrounding line profile analysis, as well as, develop a deeper understanding of the structure and dynamics of nanoscale materials.

Host: Henry Chapman – CFEL Coherent Imaging Division