

ELEMENT-SPECIFIC STRUCTURE OF NANOSIZED MATERIALS BY HIGH-ENERGY RESONANT X-RAY DIFFRACTION AND DIFFERENTIAL ATOMIC PAIR DISTRIBUTION FUNCTIONS

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High-energy X-ray diffraction (XRD) combined with atomic pair distribution function (PDF) data analysis has already proven to be very efficient in determining the 3D structure of nanosized materials. A single high-energy XRD experiment, however, yields a so-called total PDF which is a weighted sum of several contributions each reflecting the spatial correlations between a particular pair of atoms in the material. This can make difficult or ambiguous the interpretation of PDF data, especially in the case of multi-element materials. We will discuss how high-energy resonant X-ray diffraction (XRD) and differential atomic PDFs analysis can be used to characterize the atomic ordering in nanosized materials with both excellent spatial resolution and element specificity. Examples will include PtPd core-shell nanoparticles (Pt Ka edge ~ 78 keV) and nanophase BiFeO₃ (Bi Ka edge ~ 90 keV).