

# **A THEORETICAL STUDY OF X-RAY DIFFRACTION FROM NANOMATERIALS**

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X-ray diffraction is a powerful tool to study the structural parameters (size, strain, etc.) of nanomaterials. However, it still remains a challenge to interpret the diffraction pattern correctly, no matter for a powder sample or a single nanoparticle/nanodomain. In particular for the latter case, with the advance of x-ray optics, nanobeams with sub-100 nm size becomes available at synchrotron source and nanobeam diffraction emerges as an invaluable tool to explore structural changes on the nanoscale. Because of the complex incident wavefront introduced by nanofocusing optics, new data analysis methods have to be developed and there is a strong interest to fully understand the nanodiffraction pattern. Here we will present forward modeling of diffraction patterns from nanoparticles/nanodomains at mid to high energy x-ray energy. Non-planar wavefront will be incorporated into the calculation to account for the effect of focusing optics for nanobeam diffraction. We will discuss the accuracy and precision achieved by currently available techniques as well as the requirements for structural characterization at synchrotron x-ray instruments employing nanobeams.