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Advancing X-Ray Pair Distribution Function and Diffraction Capabilities at the Canadian Light Source

Wednesday 11 June 2025 10:30 (30 minutes)

A series of significant advances in our acquisition and analysis of total scattering measurements at the Brockhouse X-Ray Diffraction and Scattering Sector (BXDS) of the Canadian Light Source has enabled atomic pair distribution functions (PDF) of unprecedented quality and sensitivity along with simultaneous high-resolution powder diffraction for Rietveld analysis. We have also managed to successfully produce excellent 3D-PDFs and conducted insitu studies. An overview of the new methods and capabilities will be presented. The PDF, Rietveld and 3D-PDF methods have been applied for the structure study of polycrystalline, nanomaterials, amorphous systems, and molecules in solution. This serves as an excellent analytical tool for structure determination and phase identification for exsitu, insitu and in-operando studies.
The performance of the current BXDS beamline will be compared with estimates based on potential CLS source upgrades as well as several fourth-generation high energy x-ray sources. Options for increasing capacity and performance will be presented. This will provide a better understanding of the comparison of 3rd generation synchrotrons and 4th generation synchrotrons as sources for PDF and high energy diffraction beamlines.

Keyword-1

Synchrotron Instrumentation

Keyword-2

Pair Distribution Function

Keyword-3

X-Ray Diffraction

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