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Total scattering: science that's better than average

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Local-scale defects and disorder are essential in the development of new advanced functional materials. However, such features are often difficult to characterize and understand without suitable probes. Powder diffraction is a powerful technique for understanding atomic structures, however, Bragg peaks alone are limited to information regarding the “average” or long-range structure. The presence of local-scale disorder results in diffuse features that occur beneath and between the Bragg peaks. Hence, the characterisation of nano-scale (0.1 – 3 nm) features in functional materials demands an alternative approach.

Total scattering involves the collection of both Bragg and diffuse data over a wide Q-range. This can be Fourier transformed to generate the pair distribution function (PDF), which corresponds to an interatomic histogram of atom-atom pairs in real space. Analyzing such data can enable the development of atomic models that capture the local- and long-range structural features. Such measurements require the use of high energy x-rays and/or neutrons. With the development of the advanced diffraction and scattering beamline at the Australian synchrotron, such measurements will become viable in Australia.

This presentation will show clear-cut examples of the application of total scattering in materials chemistry. This will show the necessity for local structure analysis in developing a complete understanding of structure-property relationships.

Presenter Gender

Man

Do you wish to take part in the Student Poster Slam

Condition of submission

Yes

Students Only - Are you interested in AINSE student funding

Level of Expertise

Early Career <5 Years

Pronouns

Which facility did you use for your research

Australian Centre for Neutron Scattering

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