



Contribution ID : 18

Type : Oral

Total Scattering Measurements at the Australian Synchrotron Powder Diffraction Beamline: Capabilities and Limitations

Wednesday, 24 November 2021 12:05 (15)

The PD beamline at the Australian Synchrotron (ANSTO) consistently receives requests to carry out total scattering experiments for various materials including battery electrodes, piezoelectrics and coordination frameworks. In this study we describe the capabilities and limitations of carrying out total scattering experiments on the Powder Diffraction beamline. A maximum instrument momentum transfer of $19 \text{ \AA}^{-1}$ can be achieved. Our results detail how the pair distribution function is affected by Q_{max} , absorption, and counting time duration at the PD beamline. We also trial a variable counting time strategy using the Mythen II detector. Refined structural parameters exemplify how the PDF is affected by these parameters. Total scattering experiments can be carried out at PD although there are limitations. These are: (1) only measurements on stable systems and at non-ambient conditions is possible if the temperature is held during data collection, (2) it is essential to dilute highly absorbing samples ($\mu_R > 1$), and (3) only correlation lengths $> 0.35 \text{ \AA}$ may be resolved. A case study comparing the PDF atom-atom correlation lengths with EXAFS derived radial distances of Ni and Pt nanoparticles is also presented, which shows good agreement between the two techniques. The results here can be used as a guide for researchers considering total scattering experiments at the PD beamline.

Level of Expertise

Early Career <5 Years

Presenter Gender

Woman

Pronouns

She/Her

Which facility did you use for your research

Australian Synchrotron

Students Only - Are you interested in AINSE student funding

No

Do you wish to take part in the Student Poster Slam

No

Condition of submission

Yes

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Session Classification : Instruments & Techniques

Track Classification : Instruments & Techniques