

Benchmarking the 3D- Δ PDF using in-house X-ray sources

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The analysis of diffuse scattering from single crystals using the three-dimensional difference pair-distribution function (3D- Δ PDF) has emerged within the last decade [1] and proved useful in understanding the structure of complex thermoelectric materials such as Cu_{1.95}Se [2], metal-organic frameworks like DUT-8 [3], and battery materials [4].

Due to the weak nature of the diffuse scattering, measurements have previously been conducted at synchrotron facilities where extremely high beam flux and short wavelength make them ideal for measurements aimed at 3D- Δ PDF analysis. Recently, Schmidt *et al.* [5] showed that it was possible to perform the same analysis based on data from an in-house Rigaku Synergy-S diffractometer.

This work focuses at benchmarking the 3D- Δ PDF using a Rigaku Synergy-S diffractometer with characteristic Mo-radiation aimed at a comparison of the in-house source against its synchrotron counterpart using three selected systems. Each system was chosen to highlight different aspects of the 3D- Δ PDF. The first system, Cu_{1.95}Se contains strong diffuse scattering separated from the Bragg peaks [2], thus serving as proof of concept. Secondly, Nb_{1-x}CoSb contains weak diffuse scattering, yet still separated from the Bragg peaks [6]. Finally, we examine InTe, which combines the weak diffuse scattering with its overlap with the Bragg peaks [7] thus probing the limits of the method.

As an example, Fig. 1 shows a section of the 3D- Δ PDF for Cu_{1.95}Se measured on synchrotron and in-house, respectively. The most prominent difference is the noise near the origin of the in-house 3D- Δ PDF, which hinders part of the analysis, but for Cu_{1.95}Se, the periodicity of the 3D- Δ PDF allows an origin shift which enables the analysis using one of the nearby features.

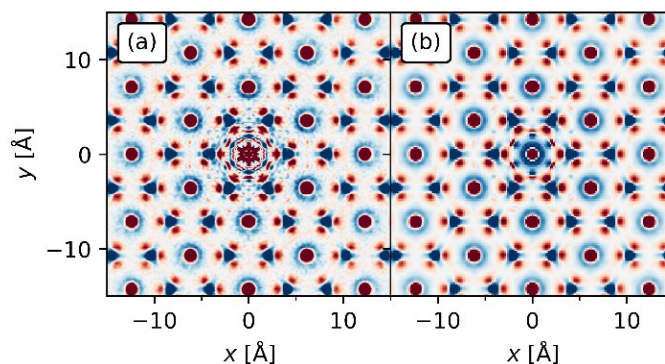


Figure 1. The 3D- Δ PDF for Cu_{1.95}Se in the $z = 0$ Å plane measured on (a) in-house, and (b) synchrotron sources.

This work shows that while in-house sources have lower resolution and lower signal-to-noise ratio compared to synchrotron sources, it is possible to analyse diffuse scattering data and reach the same conclusions. This greatly enhances the availability of the method as in-house sources are more accessible and is a great step towards the 3D- Δ PDF being a more common tool for analysis of disorder.

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