Oral Contributions

[MS27 - 03] 3D-PDF as a framework for comparing different local ordering models in single crystals. Arkadiy Simonov, Thomas Weber, Walter Steurer

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Analysis of diffuse scattering currently becomes a popular tool for investigating local order in crystalline materials. It gives detailed structural information, which can be important for a broad range of problems from predicting activity of catalyzers[1] and understanding chemistry of host-guest systems, to explaining details of atomic migration in ion-conductive materials[2], to tailoring materials with desired properties, such as ferroelectricity[3] or giant magneto-resistivity[4]. The approaches to investigate diffuse scattering vary as profoundly as the systems they try to explain. The popular methods include molecular dynamics and Monte-Carlo modelling, reverse Monte-Carlo fitting in real space, several techniques related to phonon spectra and Brillouin zone calculations in reciprocal space, as well as analytical models. Sometimes the same experiment can be described in several formalisms providing results, which are not easily comparable. In the present contribution we argue that the 3D pair distribution function (3D-PDF) may valuable as an intermediate representation for comparing various ordering models, because, firstly the PDF can be easily calculated from most of the formalisms, secondly it contains all the information that can be accessed by diffraction experiments, and thirdly the PDF is easier to interpret than raw diffuse scattering. Furthermore, the 3D-PDF provides by far more detailed information than the traditional powder diffraction based PDF method.

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