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Keywords: thermoelectrics, tellurides, defects, 7Li NMR

MS21 Structural disorder and materials' properties at ambient and non-ambient conditions

Chairs: Dmitry Chernyshov, Vaughan Gavin

MS21-O1 Lattice dynamics and elastic properties from thermal diffuse scattering

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Diffuse scattering from thermally populated phonons contains important details on the lattice dynamics. The intensity distribution of thermal diffuse scattering across reciprocal space allows for the identification and localization of phonon anomalies and naturally encodes the phonon eigenvectors [1]. In this presentation, the audience will be introduced to the theoretical background, recent developments on model calculations and the use of pertinent software for computing the intensity distribution in 3D reciprocal space [2]. Important aspects of the experimental implementation and data treatment are discussed and the methodology is illustrated by a representative set of recent examples [3-5]. I will show how distinct features in the lattice dynamics leave their footprint in the intensity distribution, such as soft and low energy phonon modes (see Figure 1), similarities in the electronic potential and symmetry relations upon phase transitions. Finally, the possibility for extracting the full elasticity tensor from thermal diffuse scattering is discussed and an outlook to application at high pressures is presented.

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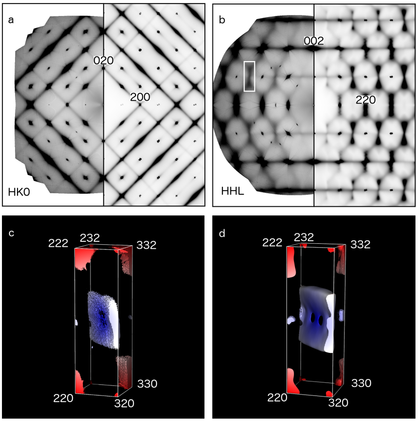

Figure 1. TDS from TiO_2 [3]. Reconstructions from experiment (left part of panels a and b) are compared to model calculations using density functional perturbation theory. (c) and (d) iso-intensity distribution of TDS in 3D around Q = (2.5 2.5 1) as obtained from experiment and calculation, respectively.

Keywords: diffuse scattering, lattice dynamics, elasticity

MS21-O2 3D Single Crystal Diffuse Scattering - Measurement and Interpretation

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The useful and interesting properties of many crystalline materials are due to crystal defects. Defects manifest themselves by diffuse scattering interspersed between the Bragg reflections. The total scattering, Bragg and diffuse, contains information on the periodic portion of the total scattering density including its chemically unreasonable parts and the nature of the underlying crystal defects as well as the correlation between them.

Nowadays reasonably accurate measurement of complete 3D total scattering is possible at synchrotrons with their high flux of X-rays and low-noise, energy discriminating pixel detectors. Several neutron scattering facilities provide stations for measuring 3D diffuse scattering patterns. Careful data processing is mandatory, especially with respect to background corrections. Diffuse data sets may contain millions to hundreds of millions of observations. Their handling and interpretation thus requires substantial computing resources.

Interpretation of such data relies primarily on two tools [1]: 1) analysis of the 3D-PDF, i.e. the Fourier Transform (FT) of the total scattering intensity. The 3D-PDF is the non-periodic Patterson function of the disordered crystal just like the FT of the Bragg intensities is the periodic Patterson function P of an ordered crystal. With a good model of the average, periodic structure usually available, the 3D-ΔPDF=3D-PDF-P is usually more informative. It represents the deviations from periodicity in terms of inter-nuclear vectors, their intensity and a between-atoms temperature factor. 2) The disordered structure may be modeled with Monte Carlo (MC) simulations constrained to match the average structure. In practice it is often useful to alternate between MC modeling and the 3D-ΔΔPDF=3D-ΔPDF(exp)-3D-ΔPDF(MC model).

The information from 3D total scattering patterns is necessarily superior to that of 1D powder patterns as is the information from 3D single crystal Bragg data compared to powder diagrams. The general comments above will be illustrated with a 3D-PDF/MC interpretation of X-ray and neutron data measured for the same compound.

[1] For a recent review see: T.R. Welberry, T. Weber, Cryst. Rev. **22** (2016) 2-78.

Keywords: Disorder, Diffuse scattering, Pair Distribution Function, Monte Carlo simulation