Poster Presentations

[MS27-P06] A 3D-ΔPDF Real Structure Study of PbTe

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Thanks to its low thermal conductivity the compound PbTe belongs to the leading thermoelectric materials. From the rock salt type average structure alone, however, its physical properties cannot be completely understood. To gain a deeper insight in the structure-property correlations of PbTe its local and long-range structure was recently studied with a broad range of methods like the powder pair distribution function (PDF) [1], inelastic neutron scattering [2,3] and molecular dynamics simulations [4]. In summary it was concluded that the structure shows local polarity, which is stimulated by phonons. In this study we investigate the temperature dependent local structure of PbTe based on single crystal diffuse scattering. High quality data from 125K up to room temperature were measured at the Swiss Light Source (beamline X06SA) using a PILATUS 6M detector. The data were analysed with the single crystal PDF (3DΔPDF) modelling program YELL [5]. Our findings fully support the previously proposed model of phonon induced local polarity. To our surprise we observed that the general appearance of the diffuse scattering does hardly change as a function of temperature. As a consequence of the smaller amplitudes of the atomic displacements only the total intensity of the diffuse scattering decreases towards lower temperatures. The profiles of the diffuse scattering are almost unchanged, however, what can be interpreted such that the correlation fields do not vary significantly within the examined temperature range. The complete 3D-ΔPDF analysis provides a detailed quantitative picture about atomic pair correlations up to distances ofabout 60Å. This not only allows a comprehensive insight into the local structure of PbTe, but also demonstrates the power of the 3D-ΔPDF method for analysing the local structure of disordered crystals.

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