Poster Presentations

[MS14-P04] Real structure of $Ge_4Bi_2Te_7$: analysis of diffuse scattering with 3D-ΔPDF.

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In addition to many different stable long-range ordered structures in the system $(GeTe)_n(Bi_2Te_3)$ [1] there are also metastable phases, which can be obtained by quenching high-temperature phases. They show pronounced real structure phenomena, similar to those known from $(GeTe)_n(Sb_2Te_3)$ thermoelectrics.[2] Single crystals of $Ge_4Bi_2Te_7$ are accessible via chemical transport reactions. They exhibit an average structure related to the NaCl type. Diffuse streaks with satellite-like maxima run along the (pseudo-)cubic <111> directions (cf. *Fig. 1*) of the fourfold twinned crystal.

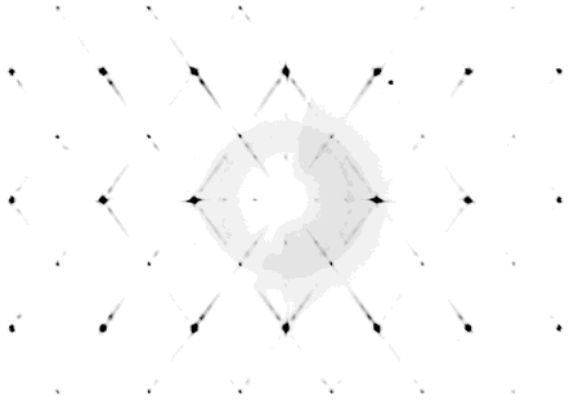

Fig. 1: hhl section of a $Ge_4Bi_2Te_7$ single crystal

These diffuse streaks arise from vacancy ordering in defect layers combined with displacements of the atoms around those layers. The 3D-ΔPDF method [3] is a powerful tool to refine the local environment of the atoms in the crystal and get quantitative information on the real structure. The refinement yields the distribution of the distances between defect layers as well as the distortions around them and the cation distribution in the layer next to the defect layer. The results match those obtained by trial-and-error modelling the features of the diffuse scattering with DIFFaX.[4]

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[4] Treacy, M. M. J., Newsam, J. M. & Deem, M. W. (1991). *Proc. Roy. Soc. Lond.* **A433**, 499-520.

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