

Poster Presentation

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Investigating anharmonicity and disorder in cadmium and zinc telluride

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CdTe and ZnTe are often referred to as II-VI semiconductors. Due to the structural and photoelectric properties and low-cost manufacturability, CdTe and ZnTe based thin films are used in the photovoltaic technology and in variety of electronic devices such as infrared, X-ray and gamma ray detectors (Eisen et al., 1998). The structure of another telluride, PbTe, has recently been reviewed and the emerging atomic disorder with temperature seems to have an indissoluble liaison with the high thermoelectric figure of merit of such promising material (Bozin et al., 2010). Deviations of the cation from its position in the ideal rock-salt structure have been probed by means of Maximum Entropy Method (MEM) calculations on Synchrotron powder X-ray diffraction data (SPXRD) (Kastbjerg et al., 2013). Motivated by the peculiar structural features in lead telluride, we investigate anharmonicity and disorder of the cations in both the zincblende structures, CdTe and ZnTe. High resolution SPXRD data at 100 K have been collected for both compounds. High energy radiation and minute capillaries have been used with the aim to minimize systematic errors on the data such as absorption and anomalous scattering. Accurate Rietveld refinements have been carried out in order to extract the best dataset of structure factors. Maximum Entropy Method calculations have hence been computed, providing the least-biased information deduction from experimental data. The disorder, anharmonicity and chemical bonding within the crystalline CdTe and ZnTe have been deeply investigated through the MEM densities and comparisons with the cation displacement in the structure of lead telluride have been established.

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