

Is the rock salt structure of SnTe so simple?

Mattia Sisti, Ellen Jensen Hedegaard, Sebastian Christensen, Niels Bindzus, Bo Brummerstedt Iversen

Center for Materials Crystallography, Department of Chemistry & iNano, Aarhus University, Langelandsgade 140, Aarhus C, DK-8000, Denmark

Tin telluride crystallizes in a rock salt structure. Recent pair distribution function investigations have revealed the formation of local dipoles between 300 K and 400 K [1]. Inelastic neutron scattering measurements and *ab initio* calculations [2] suggest that a peculiar anharmonic thermal motion is present without any off-centering on the Sn site. The possible presence of static disorder in tin telluride complements the ongoing debate on the structure of other chalcogenides such as PbX (X=S,Te) and GeTe [3-6]. The increased interest in the structure of these materials is well explained by their technologically important properties. In particular, SnTe is a thermoelectric, topological insulator and has unusual properties at the nanoscale [7]. In addition, the reported low temperature rhombohedral phase has been matter of different and sometimes discordant studies, thus making the behavior of crystalline tin telluride even more puzzling [8].

In order to shed light on the structure of tin telluride, we have collected high resolution powder and single crystal diffraction data in the range 300 K – 800 K and 20 K – 400 K, respectively. Maximum entropy calculations have been carried out in the attempt to validate any proposed structural model. Ordering of tin vacancies possibly occurs on warming which is corroborated by the appearance of multiphases, diffuse scattering and strain. The reported low temperature phase transition is strongly revised.

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