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Local Distortions in PbTe:Tl[1] TREVOR KEIBER, FRANK BRIDGES, UC Santa Cruz, BRIAN SALES, Oak Ridge National Laboratory — Lead Telluride (PbTe) is a well characterized thermoelectric material. Tl doping increases the figure of merit with a maximum at 2% Tl. Recent X-ray diffraction and total neutron scattering experiments suggest Pb moves off-center along the 100 axis as T increases. To investigate the local structure we present an Extended X-ray Absorption Fine Structure (EXAFS) analysis for 0-3% Tl concentrations at the Tl and Pb L3 edges and at the Te K edge. At 10K the local structure about Pb is well ordered, the Pb-Te (Te-Pb) pair distribution function (PDF) broadens rapidly with T. Attempts to model the increase in σ^2(T) for the Pb-Te pair (σ is the width of the PDF) with a 100 Pb off-center displacement, were not successful. However σ^2(T) for the Pb-Te pair is well described by a correlated Debye model with a low correlated Debye temperature. The Te edge shows increased disorder for the the Te-Te pair and later peaks which may be caused by a structural change around the Te atom. For Tl, the environment is distorted even at 10K within the host material. This indicates a large variation of the Tl-Te bond lengths, presumably as a result of the presence of Tl(+1). We discuss possible models for the disorder about Tl, Pb, and Te in PbTe:Tl.

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Trevor Keiber
UC Santa Cruz

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