

A Combined EXAFS and First-Principles Theory Study of Pb(1-x)Ge(x)Te

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Introduction: The narrow band-gap semiconductor Pb(1-x)Ge(x)Te has a low-temperature ferroelectric rhombohedral phase whose average structure is a distorted rock salt structure. By applying the results of first-principles theory and advanced EXAFS analytical techniques, we are able to measure various primary and secondary distortions to the local structure of this material.

Methods and Materials: Temperature dependent EXAFS measurements were performed on finely powdered Pb(1-x)Ge(x)Te with x=0.27. Data were collected at the Pb L3 edge and the Ge and Te K edges. The data from the three edges were analyzed simultaneously using theoretical fitting standards from FEFF.

Results: Our fitting model, inspired by results from first-principles calculations on this material, directly measures distortions to the structure due to subtle interatomic interactions.

Conclusions: The approach demonstrated in this work used measurement and simultaneous analysis of multiple edges, a sophisticated fitting model inspired by first-principles theory, and *ab initio* theoretical fitting standards to yield a high level of detail about the structure of this material. This approach can be applied to many other classes of technologically interesting materials.

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References: PRB 60, #21, pp. 14632-14642 (1999)