

Abstract Submitted
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Coherent Phase Stability of IV-VI Rocksalt Semiconductor Alloys¹ JEFFREY DOAK, CHRIS WOLVERTON, Northwestern University —

The creation of nanoscale precipitates via phase separation provides a mechanism for decreasing the lattice thermal conductivity of some bulk thermoelectric materials. The IV-VI semiconductor alloy systems may phase separate by either a spinodal decomposition or nucleation and growth mechanism. To better understand these phase transformations, we use first-principles density functional theory (DFT) calculations to investigate the coherent and incoherent phase stability of a series of IV-VI rocksalt semiconductor alloys (IV=Pb, Sn, Ge and VI = S, Se, Te). We use mixing enthalpies derived from calculations of special quasirandom structures (SQS), along with coherency strain energies to model the thermodynamic driving forces for incoherent and coherent phase separation. By fitting these inputs to a sub-regular mixing enthalpy model and including an ideal mixing entropy term, we calculate incoherent and coherent phase diagrams. We show the incorporation of coherency strain energies cause large depressions of the coherent spinodals for each system. The depressions are large enough that at realistic processing temperatures, the dominant precipitation mechanism of phase separation is nucleation and growth.

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Jeffrey Doak
Northwestern University

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