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**Investigating the coherent phase stability of the PbS-PbTe system using first principles calculations** WILLIAM COUNTS, CHRIS WOLVERTON, Northwestern University — Nanoscale inhomogeneities in PbS-PbTe alloys may enhance thermoelectric properties of these materials. The phase diagram and coherent spinodal are key factors controlling these nanostructured morphologies. We study the coherent phase stability of PbS-PbTe using density functional theory based calculations, a mixed-space cluster expansion, and Monte Carlo simulations. (i) Our calculations correctly reproduce the phase separating tendency of the PbS-PbTe phase diagram. (ii) Strain energy calculations show that for this rocksalt-based system (100) is the elastically hardest direction and that (111) is the softest. (iii) The formation energies for the PbS-PbTe structures are of the same order as the strain energies suggesting that strain energy will significantly depress spinodal decomposition in this system.

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