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First-principles theory of phase stability, solvus boundaries, and coherency strain in LAST (lead-antimony-silver-telluride) and in other doped $AgSbTe_2$ thermoelectric alloys[1] SERGEY V. BARABASH, VIDVUDS OZOLINS, UCLA, CHRIS WOLVERTON, Northwestern University — Bulk telluride alloys are promising thermoelectrics [e.g. the figure of merit (ZT) of LAST ($AgPb_mSbTe_{2+m}$) alloys was reported* to exceed $ZT\sim2$]. Recent theoretical examination+ found that precipitation of ordered $AgSbTe_2$ phases in rocksalt PbTe likely contributes to the high ZT of LAST, and predicted that the isoplethal PbTe-$AgSbTe_2$ phase diagram includes highly asymmetric miscibility gap. Here we generalize that analysis by first launching a search for *unknown* (Ag,Pb,Sb)Te non-rocksalt phases (those deviating from the 1:1 cation:anion ratio), and second by presenting an extended analysis of the solubility limits for alloying $AgSbTe_2$ with PbTe and other tellurides. In particular, we find that the large asymmetry of the PbTe-$AgSbTe_2$ miscibility gap shares a common physical origin with the substitutional site preference for Pb in ordered $AgSbTe_2$, and that during coherent precipitation, the coherency strain increases the solubility limits in PbTe-$AgSbTe_2$ by a factor of $\sim$2 relative to the predicted+ unstrained bulk values. *K.F. Hsu *et al.*, Science **303**, 818 (2004). +S.V.Barabash *et al.*, Phys.Rev.Lett. **101**, 155704

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