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Large Enhancements in Thermopower and Electrical Conductivity in Nano-structured Half-Heusler Alloys ALEXANDER PAGE, University of Michigan, ANTON VAN DER VEN, University of California Santa Barbara, PIERRE POUDEU, CTIRAD UHER, University of Michigan — Recent improvements have often been made to thermoelectric materials by adding nano-structures in order to scatter heat carrying phonons, however, the reduction in thermal conductivity is accompanied by large drops in the electrical conductivity caused by mobility reductions. In this work we show that Half-Heusler (HH) alloys can be combined with nano-scale Full-Heusler (FH) inclusions to simultaneously improve the power factor and reduce thermal conductivity. HH structures are of the form MNiSn and MCoSb (M= Ti, Zr, or Hf) and the FH counterparts are created by filling the vacancies on the Ni or Co planes respectively, giving MNi_2Sn and MCo_2Sb. Experimental results show FH nano-inclusions were coherently integrated into the matrix HH material resulting in enhanced ZT which is attributed to energy filtering effects that occur at the HH-FH grain boundaries as well as moderate reductions in thermal conductivity by nano-inclusion phonon scattering. *Ab Initio* calculations, in combination with a cluster expansion, are used to test the stability of FH structures in HH matrix and create thermodynamic pseudo-binary phase diagram for MNiSn-MNi2Sn compositions, elucidating the possibilities for future approaches to enhance ZT.

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