Highlights

RESEARCH AREA 1 - **Superconductors and Innovative materials for Energy and Environment** - 2022

"Roles of Defects and Sb-doping in the Thermoelec-tric Properties of Full-Heusler Fe_2TiSn"

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The potential of Fe_2TiSn full-Heusler compounds for thermoelectric applications has been suggested theoretically, but not yet grounded experimentally, due to the difficulty of obtaining reproducible, homogeneous, phase pure and defect free samples. In this work, we study $Fe_2TiSn_{1-x}Sb_x$ polycrystals (x from 0 to 0.6), fabricated by high-frequency melting and long-time high-temperature annealing. We obtain fairly good phase purity, homogeneous microstructure and good matrix stoichiometry. Although intrinsic p-type transport behavior is dominant, n-type charge compensation by Sb doping is demonstrated. Calculations of formation energy of defects and electronic properties carried out in the density functional theory formalism reveal that charged iron vacancies V_{Fe}^{2-} are the dominant defects responsible for the intrinsic p-type doping of Fe_2TiSn in all types of growing conditions except Fe-rich. Additionally, Sb substitutions at Sn site give rise either to Sb_{Sn}, Sb_{Sn}^{1+} which are responsible for n-type doping and magnetism (Sb_{Sn}) or to magnetic Sb_{Sn}^{1-} which act as additional p-type dopants. Our experimental data highlight good thermoelectric properties close to room temperature, with Seebeck coefficients up to 56 µV/K in the x=0.2 sample and power factors up to 4.8×10^{-4} W m^{-1} K^{-2} in the x=0.1 sample. Our calculations indicate the appearance of a pseudogap in Ti-rich conditions and large Sb doping, possibly improving further the thermoelectric properties.

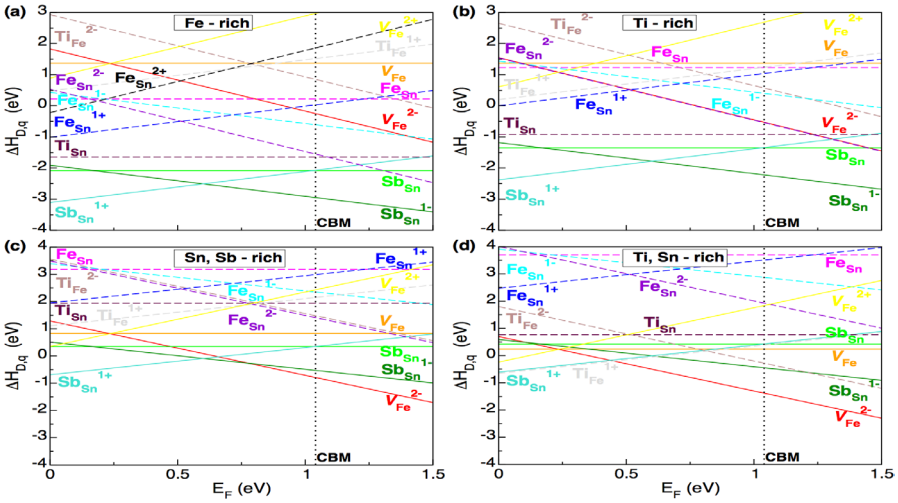

Fig. 1: Fermi energy dependence of formation energy of different types of atomic defects

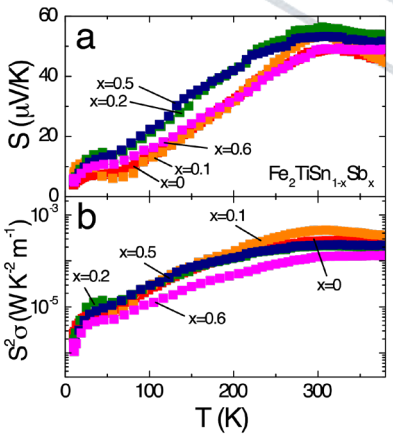

Fig. 2: Seebeck coefficient (a) and thermoelectric power factor (b) measured in $Fe_2TiSn_{1-x}Sb_x$ (x = 0.0, 0.1, 0.2, 0.5 and 0.6) samples.