Theoretical Modelling of Thermoelectric Properties of $Fe_2Ti_{1-x}V_xSn$ Heusler Alloys

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Fe_2TiSn is a full-Heusler alloy with 24 valence electrons per formula unit. Its electronic properties, thermal and chemical stability, relatively low cost of constituent elements make it a potential thermoelectric material for practical applications for conversion of waste heat to electricity. Doping Fe_2TiSn with vanadium can improve thermoelectric figure-of-merit ZT

$$ZT = \frac{S^2 \sigma T}{k_{el} + k_{ph}}; \quad S^2 \sigma = PF$$

Where S means Seebeck coefficient, σ is the electric conductivity, T is the temperature, k_{el} and k_{ph} is the electronic and phononic thermal conductivity. Priduct of S^2 and σ is called power factor PF. Previous theoretical calculations show maximal power factor values of Fe_2TiSn at delta VEC (Valence electron count per formula unit) = 0.06 [1]. In this work, various doping level was modelled by substituting Ti atom by V in model structure cells with different size. The thermoelectric properties of $Fe_2Ti_{1-x}V_xSn$ (x=0, 0.0625, 0.094, 0.125, 0.25) were examined using first-principles density functional theory in the plane-waves basis set and semi-classical Boltzmann transport theory. Our results testify previous theoretical calculations and confirm, that $Fe_2Ti_{1-x}V_xSn$ (x=0.0625, 0.094, 0.125, 0.25) alloy has a big potential to realize a higher figure-of-merit (ZT) value, compared to conventional Fe_2TiSn (Fig. 15).
According to previous [1] and present theoretical results polycrystalline ingots of $Fe_2Ti_{1-x}V_xSn$ ($0 \le x \le 0.2$) were prepared by arc melting method in protective argon atmosphere. The obtained ingots were annealed in vacuum at 1073 K for 10 h. X-ray diffraction revealed that all the alloys crystallize in the $L2_1$ Heusler structure.

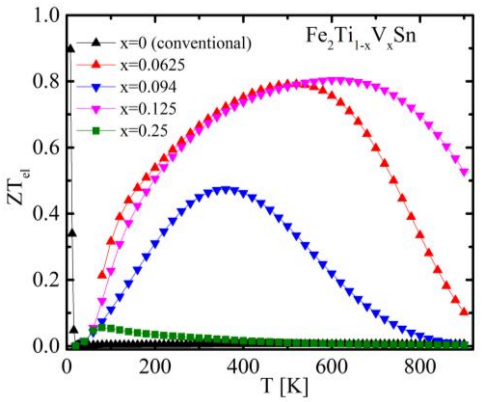

Fig. 15 Calculated dependence of electronic figure-of-merit ZT ($k_{ph} = 0$) on temperature for $Fe_2Ti_{1-x}V_xSn$ (x=0, 0.0625, 0.094, 0.125, 0.25)

[1] S. Yabuuchi, M. Okamoto, A. Nishide, Y. Kurosaki, J. Hayakawa, Appl. Phys. Express **6**(2), 025504 (2013).