ELECTRON TRANSPORT PROPERTIES CALCULATED FROM FERMI SURFACE AND BOLTZMANN EQUATION IN DISORDERED HALF-HEUSLER THERMOELECTRICS

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9.7 cm

The half-Heusler phases still belong to an interesting class of thermoelectric materials. The Green function Korringa-Kohn-Rostoker methodology [1,2] with the coherent potential approximation was used to calculate electronic, magnetic and transport properties in chemically disordered compounds that exhibit metal-semiconductor-metal crossovers. The transport function within the Boltzmann approach, was originally implemented and calculated with the use of velocities and life-times of electrons determined on the complex energy Fermi surfaces. The computed Onsager coefficients allowed to derive electron transport coefficients as thermopower or electrical resistivity. In particular the aforementioned procedure was applied to (Ti,Zr,Hf)Fe_{1-x}(Ni,Pt)$_x$Sb compounds that experimentally revealed tunable electron transport properties with high Seebeck coefficient and metal-semiconductor-metal crossovers accompanied by a change of carrier types [3]. Additionally the critical crossover concentrations was compared with experimental datas. One of us (K.K.) acknowledges the partial support by the EU Human Capital Operation Program, Polish Project No. POKL.04.0101-00-434/08-00.

[1] Bansil et al., Phys. Rev. B 60, 13396 (1999).
[2] Stopa et al., J. Phys.: Condens. Matter 16, 4921 (2004).
[3] Tobola et al., J. Alloys Compd. 383 (2004) 328.

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