SEMICONDUCTING PROPERTIES OF DISORDERED HALF-HEUSLER SYSTEMS

J. Toboła[a], G. Venturini [b] and S. Kaprzyk[a]

[a]Faculty of Physics and Nuclear Techniques, University of Mining and Metallurgy, 30-059 Cracow, Poland

[b]Laboratoire de Chimie du Solide Mineral, Université H. Poincaré, Vandoeuvre-les-Nancy, 54042 Nancy Cedex, France

9.7 cm

Recently, a composition induced metal-semiconductor-metal crossover has been detected in the $Fe_{1-x}Ni_xTiSb$ half-Heusler system using resistivity and thermopower measurements and supported by electronic structure computations based on the KKR-CPA method [1]. Such an unusual behavior is also expected in other disordered half-Heusler phases possessing the critical number of the valence electrons.
We present results of electronic structure calculations on $Fe_{1-x}Pt_xZrSb$, $Ru_{1-x}Ni_xZrSb$ and $Ru_{1-x}Pd_xZrSb$ which are isoelectronic to the aforementioned system. The onset of semiconducting state, when alloying parent compounds (metals), is detected through a remarkable modification of density of states as a function of composition. Moreover, a shift of the Fermi level (E_F) from valence to conduction states for $x \approx 0.5$, should have an apparent effect on conductivity and thermopower behavior.
The appearance of the energy gap at E_F in the disordered alloys is also in line with previous studies on ordered half-Heusler systems, which revealed a high propensity for forming bandgaps in the compounds having 18 valence electrons.

[1] J. Toboła et al., Phys. Rev. **B** 64, 155103 (2001).

13.4 cm

Subject category :

7. Computations of Electronic Band Structures

Presentation mode :
oral

Corresponding author :
J. Toboła

Address for correspondence :
1. Faculty of Physics and Nuclear Techniques, AGH
Al. Mickiewicza 30, 30-059 Cracow, Poland
2. Laboratoire de Physique des Materiaux, Ecole des Mines
Parc du Saurupt, 54042 Nancy Cedex, France

Email address :
tobola@ftj.agh.edu.pl