THE ELECTRICAL CONDUCTIVITY IN THE OFF-STOICHIOMETRIC HEUSLER Fe_2VX (X=Al, Ga)

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9.7 cm

The Fe_2VX (X=Al, Ga) Heusler compounds exhibit several properties uncommon among the 3d-transition metal intermetallic compounds. The most intriguing is the semiconductor-like behavior of the electrical resistivity with simultaneous anomalously large value of electronic specific coefficient γ. The calculated electronic structure of the Fe_2VAl characterizes a deep, 0.5 eV wide, pseudo-gap centered at Fermi level (ε_F). Our recent electronic structure calculations of the off-stoichiometric $Fe_{(2+y)}V_{(1-y)}X$ ($y = \pm 0.06$) compositions have proved the existence of the narrow band located just at ε_F. In the non-magnetic state of the $y > 0$ composition the band appeared to be the almost fully occupied upper Hubbard band of the d-e_g states of the impurity Fe atoms. The presence of the band explains the large value of the γ coefficient. It may also response for the negative value of the temperature coefficient of the DC-resistivity. To investigate this we considered the two-band model of the strongly correlated narrow band coupled by the hybridization interaction with the quasi-free electron band. The model was solved by the CPA approach within the Alloy Analogy approximation and the Kubo-Greenwood formula for the DC-conductivity was applied. The calculated temperature dependence of the DC-resistivity qualitatively agree with the measured one.

13.4 cm

Subject category :

3. Transition Metals, Alloys and Compounds

Presentation mode :
poster

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