Materials Science-Poland, Vol. 25, No. 2, 2007

Electronic structure of Fe_2VGa

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We present the band structure calculations on the Heusler alloy Fe_2VGa which shows a pseudogap at the Fermi level. The compound is found to be nonmagnetic. We observed, however, that an atomic disorder which has been experimentally observed can lead to the behaviour characteristic of the heavy-Fermion compounds. The antisite Fe defects locate the d states forming a narrow d-band at the Fermi level.

Key words: *electronic structure; strong electron correlations*

1. Introduction

The physics of d-electron intermetallic compounds with electronic gaps or pseudogaps at the Fermi level continues to attract attention. This gap (pseudogap) in materials containing localized magnetic orbitals may be due to hybridization or Kondo -type singlet formalism (e.g., [1]).

Recently, the Heusler-type Fe_2VAl [2] and Fe_2TiSn [3] compounds have been discussed as possible d-Kondo insulators of the FeSi-type [4] due to their unusual electric transport and thermodynamic properties. Namely, the electrical resistivity of both compounds exhibits semiconducting behaviour and the low-*T* specific-heat data revealed an unusual upturn in C/T, commonly observed in most heavy fermion systems. From the band-structure calculations and infrared studies it follows, however, that Fe_2VAl [5] and Fe_2TiSn [6] are semimetals with a pseudogap at the Fermi level. In our recent work [7], we discussed the low-*T* properties of these compounds based on the Kimball–Falicov model [8] well describing the temperature characteristics attributed to the narrow d-antisite band, strongly correlated and located at the Fermi level.

Similarly, Fe_2VGa is predicted from the band structure calculations to be semimetallic [9, 10] and nonmagnetic. However, in some Fe_2VGa samples characteristic features of superparamagnetic glass due to the presence magnetic defects are reported (e.g., in [11]). It has been suggested that the wrong-site Fe atoms on V sites (Fe_{AS}

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antisite) are magnetic and can play a significant role in the magnetism of this compound. We therefore present our LAPW calculations on the ordered Fe_2VGa, and on the disordered one, in which an atomic disorder results from the Fe/V site exchange. Our calculations show that the antisite defects locate the d-states at the Fermi level, resulting in formation of a narrow d-band, but the system is nonmagnetic. However, magnetic Fe-defects are expected for stronger atomic disorder.

2. Results and discussion

In our investigations, we used FP-LAPW (Wien2k) code, with GGA96 type gradient corrections [12]. We performed calculations for base Fe_2VGa compound, and also for a 2×1×1 supercell, where two Fe atoms were replaced by two V atoms and vice versa. Atomic radii were chosen 2.32 Å for Fe and V and 2.2 Å for Ga. We used 816 *k*-points in reduced Brillouin zone for the calculations of base compound and 162 *k*-points for the supercell calculations.

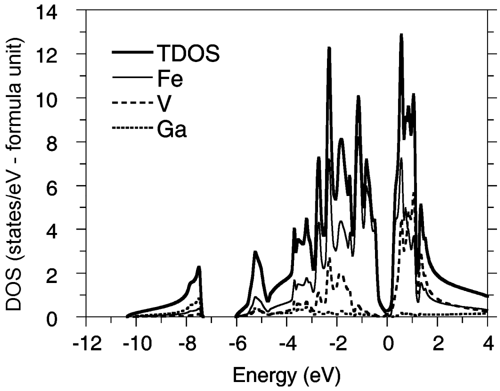

Fig. 1. Total density of states calculated for Fe_2VGa. Also, the partial total DOSs for Fe, V and Ga components are shown

In Figure 1, we present numerical calculations of the electronic densities of states (DOS) of the ordered Fe_2VGa compound. Also shown in the figure are the total DOSs of Fe, V and Ga. The electronic bands exhibit a pseudogap at the Fermi level with a small value of the total DOS of about 0.25 states/eV-formula unit. In our calculations, Fe_2VGa is nonmagnetic. To better understand the properties of real Fe_2VGa crystals, exhibiting strong atomic disorder, we also investigated the electronic structure of the Fe_2VGa alloy with one Fe atom occupying the V site. The results of our calculations are presented in Figs. 2a–d. The total DOS has a pseudogap located ~0.2 eV above the Fermi level and a sharp and narrow peak in the DOS just at ε_F. The DOS of this peak is composed mainly of the Fe_{AS} d-states of iron defects occupying the V sites (the inset in Fig. 2b). V defects have similar sharp and narrow d-electron peaks in the DOS (Fig. 2c). However, Fe_2VGa in our calculations is again nonmagnetic. Our recent calculations have shown that this narrow d-band originating from the impurity Fe atoms is responsible for the unusual temperature dependence of heavy Fermi-like behaviours observed either in Fe_2VAl [2] or in Fe_2TiSn [3]. The nature of the physics in the both Heusler alloys seems to be similar to that in Ce and U compounds, analyzed [7] in a many-body investigation along the line described by Liu [8]. Another explanation of the unusual low-temperature dependences of the specific heat can be discussed on the base of the spin fluctuation theory.

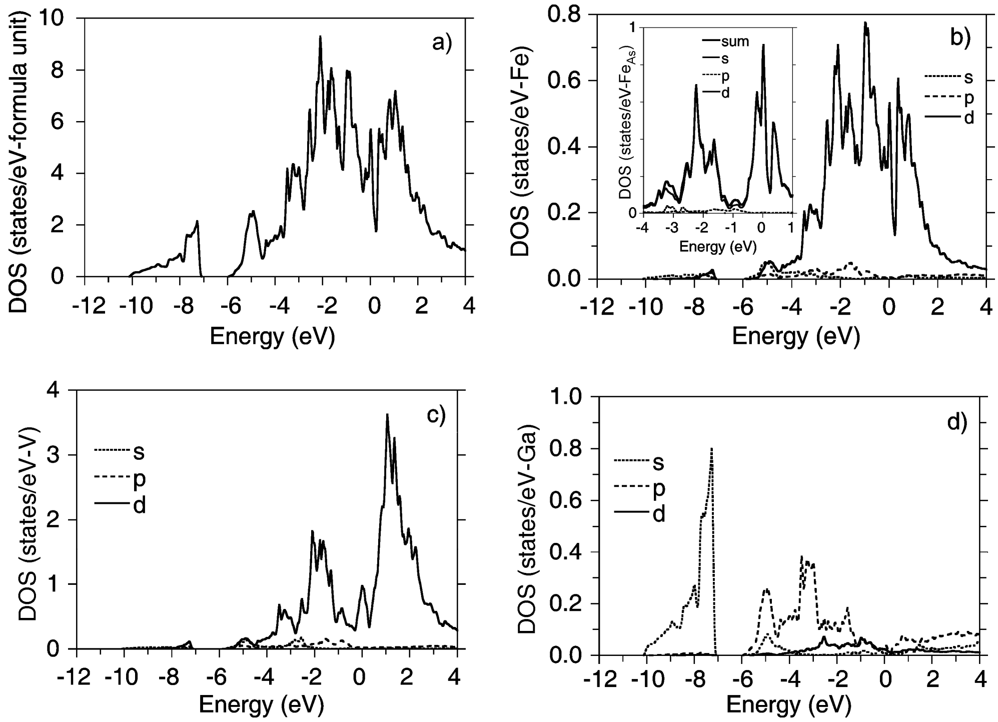

Fig. 2. The total DOS calculated for the disorder Fe_2VGa alloy, where one Fe atom occupies the V atomic position (a) and partial DOSs for s, p and d states of Fe in the disordered Fe_2VGa; the inset shows the DOSs of the Fe_{AS} defects, occupying the V sites (b); partial DOSs in Fe_2VGa (c), partial Ga DOSs in Fe_2VGa (d)

The heavy Fermi-like behaviour has not been, however, observed in the Fe_2VGa alloy probably because of strong atomic disordering, which can lead to weak super-paramagnetism, recently observed in the magnetic susceptibility experimental data [11]. The problem of magnetic/nonmagnetic ground state properties of the Fe_2VGa alloy is expected to be investigated experimentally soon.

Acknowledgements

The authors thank the Ministry of Science and Higher Education for financial support from Projects Nos. 1 P03B 052 28 and 1 P03B 094 30. We also acknowledge the Grant No. 1 PO3B 094 30 of the Ministry of Science and Information Technology.

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Received 7 May 2006
Revised 1 September 2006