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APPLICATION OF THE POLARONIC HEAVY FERMION APPROACH TO THE PROPERTIES OF THE $Fe_{2+x}V_{1-x}Al$ ALLOYS*

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The non-Fermi liquid behaviour of the Heusler-type $Fe_{2+x}V_{1-x}Al$ alloys was investigated with the use of *ab initio* and many-body methods. Calculations have shown that the narrow d band originating from the impurity Fe atoms is responsible for the unusual temperature dependence of different physical properties of these materials.

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1. Introduction

Experimental investigations [1] have shown that several properties observed in the Fe_2VAl Heusler compound and $Fe_{2+x}V_{1-x}Al$ ($x \geq 0$) alloys resemble those of the non-magnetic narrow-gap semiconductor FeSi known as the d-electron "Kondo" insulator [2]. The most intriguing, supporting the classification of $Fe_{2+x}V_{1-x}Al$ materials to the group of the $3d$ heavy fermion materials, are: the semiconductor-like behaviour of the resistivity in the paramagnetic state; the large (compared with the normal metal) value of the low temperature electronic specific heat coefficient γ showing an upturn at temperatures below few Kelvins and no traces of the energy-gap on the valence-band XPS spectrum. Our recent *ab initio* electronic structure calculations [3] have shown that the anti-site (AS) defects of Fe atoms at nominaly V positions of the Fe_2VAl compound (hereafter denoted as Fe^{β})

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give rise to the narrow resonance peak in the DOS located at Fermi level ε_F. In the paper we present the results for the temperature dependence of the electronic specific heat, resistivity and thermoelectric power calculated for the off-stoichiometric Fe_2VAl within the many-body approach derived by Liu [4] for heavy-electron systems.

2. Calculations and results

The electronic structure calculations [5] have shown that the Fe_2VAl compound is semi-metallic and non-magnetic having the band-structure with the $\sim 0.5\,eV$ wide pseudogap located symmetrically around the ε_F. Our recent electronic structure calculations [3] performed with the use of the approximate TB-LMTO method of Andersen *et al.*, [6] and verified within the more accurate FP-LAPW method (WIEN97 code) [7] have proved that in the concentration range $0 < x < 0.5$ the Fe^{β} defects in the non-magnetic $Fe_{2+x}V_{1-x}Al$ give rise to the narrow, strongly correlated d-like band located just at the Fermi level (ε_F). The spin-polarized calculations have shown that the Fe^{β} atoms together with the surrounding Fe atoms form the magnetic clusters (with effective moment of 3.5–4 μ_B) embedded in the non-magnetic host. Fig. 1a shows the total DOS for the $Fe_{2.06}V_{0.94}$ with the partial d-DOS

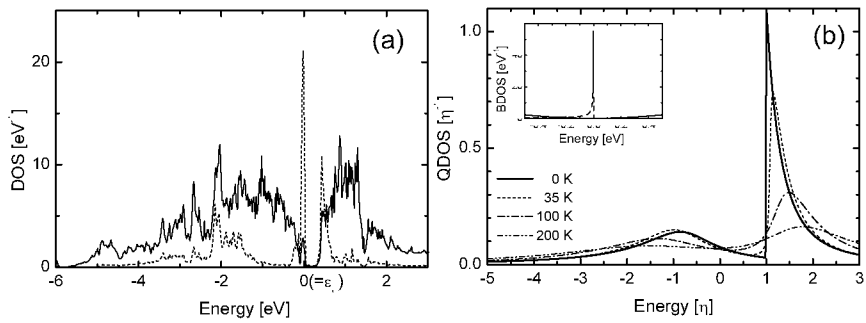

Fig. 1. (a) Total DOS for the nonmagnetic $Fe_{2.06}V_{0.94}$ (solid line) and partial Fe^{β} DOS (dash line). (b) The quasiparticle DOS in the vicinity of ε_F at different temperatures ($\eta = 0.0087$ eV). Inset shows the model Bloch-DOS of the c-like (very flat parabola) and d-like (sharp peak) electrons.

of the Fe^{β} atoms (dash line) calculated by means of the TB-LMTO method. The narrow band located just at ε_F is composed mainly of Fe^{β}-d states with e_g symmetry. The Fe^{β}-t_{2g} states form the wide band in the energy range of -4 to $-1\,eV$ and the sharp structure above ε_F. In the whole energy range the DOS is dominated by the contributions from the d-states of transition metal atoms. Except the energy region near the ε_F the shape of the DOS is almost the same as calculated for stoichiometric Fe_2VAl [5]. In the vicinity of ε_F the calculated DOS structure of the off-stoichiometric Fe_2VAl resembles

that of the heavy-fermion (mixed valent) f-electron systems with the Fermi level pinned at an energy where the narrow f-band forms. Based on that similarity we guess that the peculiar properties of the Fe_2VAl are due to the Fe^{β} defects and may have the same physical origin as that proposed for heavy-fermion f-electron systems.

One of the approach used in the description of the non-Fermi liquid behaviour of the heavy-fermion systems, based on the polaronic effects, was derived by Liu [4]. In application to our system of Fe_2VAl with Fe-AS defects the assumptions of the approach can be formulated as follows. The d-e_g electrons localized at Fe^{β} atoms (hereafter denoted as d electrons) can propagate and participate in the transport only via the hybridization with the states of the broad conduction band (c-electrons). When the d-e_g electron leaves the Fe^{β} site the remaining hole, attracting the conduction electrons, forms the polaron (the accompanying dynamical processes were discussed in details in [4, 8]). The corresponding Hamiltonian reads [4]

$$H = \sum_{\boldsymbol{k}\sigma} \varepsilon^{(c)}_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \varepsilon^{(d)} \sum_{i,\sigma} d^{\dagger}_{i\sigma} d_{i\sigma} - U_{cd} \sum_{i,\sigma\sigma'} \sum_{\boldsymbol{k},k'} d_{i\sigma} d^{\dagger}_{i\sigma} c^{\dagger}_{\boldsymbol{k}\sigma'} c_{\boldsymbol{k}'\sigma'} \mathrm{e}^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_i} + V \sum_{i\boldsymbol{k}\sigma} \left(c^{\dagger}_{\boldsymbol{k}\sigma} d_{i\sigma} \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} + \mathrm{h.c.} \right) , \quad (1)$$

where the U_{cd} term stands for the d-hole–c-electron Coulomb attraction, and the V term is the c–d hybridization. First two terms represent the c-electron kinetic energy and the d-electron atomic energy, respectively. The c-band quasiparticle spectrum is determined from the poles of the c-electron Green function: $\omega - \varepsilon_k - V^2 G_d(\omega) = 0$ with the d-electron Green function defined as $G_d(\omega) = \int \frac{S_d(\omega')d\omega'}{\omega-\omega'}$. The ground-state form of the S_d function was assumed in the shape proposed in [4] and is shown in the inset of Fig. 1. At finite temperatures the temperature dependent S_d function yields the Dyson equation for the c-band quasiparticle spectrum in the form [4]

$$\omega - \varepsilon^{(\mathrm{c})}_{\boldsymbol{k}} = \frac{W}{4\Gamma(\alpha)} \left[\frac{\beta}{\pi}\right]^{\alpha-1} \frac{\mathrm{e}^{\beta x} + \mathrm{e}^{-i\pi\alpha}}{\cosh(\beta x) + \cos(\pi\alpha)} \int_0^{\beta} \mathrm{e}^{-\tau x} \left[\sin\left(\frac{\pi\tau}{\beta}\right)\right]^{\alpha-1} d\tau ,$$

where $\beta = (k_{\mathrm{B}}T)^{-1}$, $x = (\omega - \varepsilon^d)/\eta$. The energy $\eta \left(= [2\pi V^2 A \csc(\pi\alpha)/W]^{\frac{1}{\alpha}}\right)$ determines the energy scale of the model and depends on the interaction strengths V, U_{cd} ($\alpha \propto U_{cd}$) and c-band width W. In the presented investigations the c-electron Bloch-DOS was used in the form of flat parabola simulating that of the Fe_2VAl near the ε_{F}. The position of the atomic d-level $\varepsilon^d = 0$ was assumed and the c–d hybridization $V = 0.1$ eV was used. The value of the α was taken close to that used by Liu [4]. For the calculations of the electronic specific heat (C_{el}), thermoelectric power (TEP) and resistivity we used the formulae given in [4].

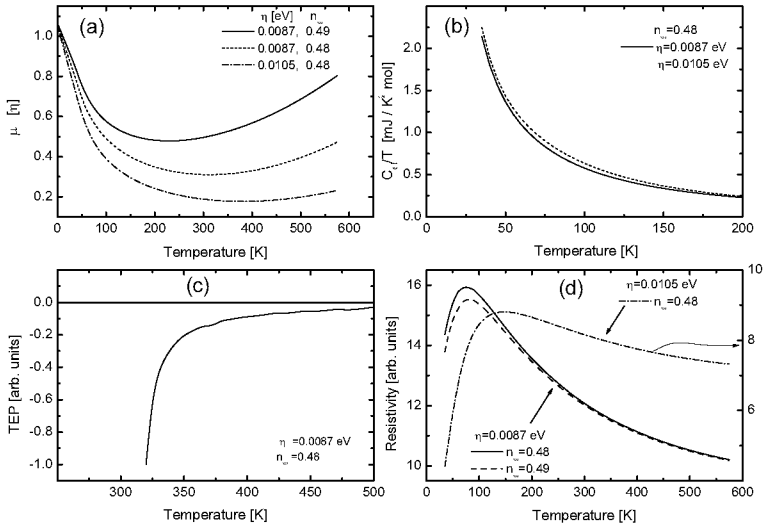

Fig. 2. Temperature dependence of: (a) — chemical potential; (b) — electronic specific heat coefficient γ; (c) — TEP; (d) — resistivity.

3. Conclusions

Fig. 2 collects the temperature variation of different calculated quantities. The calculated temperature dependences of γ, TEP and resistivity reproduce qualitatively those observed in the paramagnetic off-stoichiometric Fe_2VAl. It can be concluded that the narrow d-e_g band due to Fe^{β} AS atoms and the polaronic effects can be the origin of the unusual properties of the $Fe_{2+x}V_{1-x}Al$ materials.

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