# 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<sub>2</sub>VAl Heusler compound and Fe<sub>2+x</sub>V<sub>1-x</sub>Al ( $x \ge 0$ ) 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<sub>2+x</sub>V<sub>1-x</sub>Al materials to the group of the 3*d* 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  $\gamma$  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 nominally V positions of the Fe<sub>2</sub>VAl compound (hereafter denoted as Fe<sup> $\beta$ </sup>)

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give rise to the narrow resonance peak in the DOS located at Fermi level  $\varepsilon_{\rm F}$ . 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<sub>2</sub>VAl 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<sub>2</sub>VAl compound is semi-metallic and non-magnetic having the band-structure with the ~ 0.5 eV wide pseudogap located symmetrically around the  $\varepsilon_{\rm F}$ . 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<sup> $\beta$ </sup> defects in the non-magnetic Fe<sub>2+x</sub> V<sub>1-x</sub> Al give rise to the narrow, strongly correlated *d*-like band located just at the Fermi level ( $\varepsilon_{\rm F}$ ). The spin-polarized calculations have shown that the Fe<sup> $\beta$ </sup> atoms together with the surrounding Fe atoms form the magnetic clusters (with effective moment of  $3.5-4 \mu_{\rm B}$ ) embedded in the non-magnetic host. Fig. 1a shows the total DOS for the Fe<sub>2.06</sub> V<sub>0.94</sub> with the partial *d*-DOS



Fig. 1. (a) Total DOS for the nonmagnetic Fe<sub>2.06</sub>V<sub>0.94</sub> (solid line) and partial Fe<sup> $\beta$ </sup> DOS (dash line). (b) The quasiparticle DOS in the vicinity of  $\varepsilon_{\rm F}$  at different temperatures ( $\eta = 0.0087 \, {\rm eV}$ ). Inset shows the model Bloch-DOS of the *c*-like (very flat parabola) and *d*-like (sharp peak) electrons.

of the Fe<sup> $\beta$ </sup> atoms (dash line) calculated by means of the TB-LMTO method. The narrow band located just at  $\varepsilon_{\rm F}$  is composed mainly of Fe<sup> $\beta$ </sup>-d states with  $e_{\rm g}$  symmetry. The Fe<sup> $\beta$ </sup>- $t_{2\rm g}$  states form the wide band in the energy range of -4 to -1 eV and the sharp structure above  $\varepsilon_{\rm F}$ . 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  $\varepsilon_{\rm F}$  the shape of the DOS is almost the same as calculated for stoichiometric Fe<sub>2</sub>VAl [5]. In the vicinity of  $\varepsilon_{\rm F}$  the calculated DOS structure of the off-stoichiometric Fe<sub>2</sub>VAl 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<sub>2</sub>VAl are due to the Fe<sup> $\beta$ </sup> 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<sub>2</sub>VAl with Fe-AS defects the assumptions of the approach can be formulated as follows. The d- $e_g$ electrons localized at Fe<sup> $\beta$ </sup> 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<sup> $\beta$ </sup> 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]

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

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]

$$\omega - \varepsilon_{\boldsymbol{k}}^{(c)} = \frac{W}{4\Gamma(\alpha)} \left[\frac{\beta}{\pi}\right]^{\alpha - 1} \frac{e^{\beta x} + e^{-i\pi\alpha}}{\cosh(\beta x) + \cos(\pi\alpha)} \int_{0}^{\beta} e^{-\tau x} \left[\sin\left(\frac{\pi\tau}{\beta}\right)\right]^{\alpha - 1} d\tau ,$$

where  $\beta = (k_{\rm B}T)^{-1}$ ,  $x = (\omega - \varepsilon^d)/\eta$ . 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<sub>2</sub>VAl near the  $\varepsilon_{\rm F}$ . 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  $\alpha$  was taken close to that used by Liu [4]. For the calculations of the electronic specific heat (C<sub>el</sub>), 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  $\gamma$ ; (c) — TEP; (d) — resistivity.

#### 3. Conclusions

Fig. 2 collects the temperature variation of different calculated quantities. The calculated temperature dependences of  $\gamma$ , TEP and resistivity reproduce qualitatively those observed in the paramagnetic off-stoichiometric Fe<sub>2</sub>VAl. It can be concluded that the narrow  $d-e_{\rm g}$  band due to Fe<sup> $\beta$ </sup> AS atoms and the polaronic effects can be the origin of the unusual properties of the Fe<sub>2+x</sub>V<sub>1-x</sub>Al materials.

# REFERENCES

- Y. Nishino, M. Kato, S. Asano, K. Soda, M. Hayasaki, U. Mizutani, *Phys. Rev. Lett.* **79**, 1909 (1997); M. Kato, Y. Nishino, U. Mizutani, S. Asano, *J. Phys.: Condens. Matter* **12**, 1769 (2000). S. Nishigori, Y. Yamada, T. Ito, H. Abe, A. Matsushita, *Physica B* **281**, 686 (2000).
- [2] Z. Schlesinger, Z. Fisk, H.T. Zhang, M.B. Maple, J.F. DiTusa, G. Aeppli, *Phys. Rev. Lett.* **71**, 1748 (1993).
- [3] J. Deniszczyk, W. Borgieł, Acta Phys. Pol. A 98, 551 (2000).
- [4] S.H. Liu, Phys. Rev. B37, 3542 (1988); S.H. Liu, Physica B 240, 49 (1997).
- [5] D.J. Singh, I.I. Mazin, Phys. Rev. B57, 14352 (1998).
- [6] O.K. Andersen, O. Jepsen, Phys. Rev. Lett. 53, 2571 (1984).
- [7] P. Blaha, K. Schwarz, P. Sorantin, S.B. Trickey, Comput. Phys. Commun. 59, 399 (1990).
- [8] G.D. Mahan, Phys. Rev. 163, 612 (1967); P.W. Anderson, Phys. Rev. Lett. 18, 1049 (1967); P. Nozières, C.T. De Dominicis, Phys. Rev. 178, 1097 (1969).