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ScienceDirect
Physica B 403 (2008) 1408–1410
PHYSICA B
www.elsevier.com/locate/physb

Functional integral calculation of local magnetic moments at Ta impurities embedded in XFe_2 (X = Gd, Yb) compounds: Temperature dependence

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Abstract

In this work, we study the systematics, at finite temperature, of the formation of local magnetic moments at a Ta impurity diluted in intermetallic Laves phases compounds XFe_2 (X = Gd, Yb). We use an extended two-coupled sublattices Hubbard Hamiltonian, to describe the Laves phases host. The d–d electronic interaction is treated via a functional integral approach in the quasi-static saddle point approximation. Temperature dependent pressure effects are included considering induced electron–phonon interaction which renormalizes the pure electron hybridization. The calculated magnetic hyperfine fields related to the obtained local magnetic moments, are in a quite good agreement with available experimental data.

PACS: 71.20.Lp; 75.10.Lp; 75.20.Hr

Keywords: Intermetallic compounds; Magnetic hyperfine fields; Impurities

In this work we study, at finite temperature, the formation of the local magnetic moment and the systematics of the magnetic hyperfine fields at a Ta impurity diluted on the X site of the Laves phase intermetallic compounds XFe_2 (X = Gd, Yb). Experimental data [1,2] show that Ta impurity diluted in the XFe_2 intermetallic hosts enters in the X site. In order to calculate the magnetic properties of the XFe_2 intermetallic hosts, we use a two sublattice Hamiltonian, describing a subsystem of itinerant d-electrons coupled with localized f-spins of rare earth ions [3]. One has

$$H = \sum_{l\sigma} \varepsilon_0^X d_{l\sigma}^\dagger d_{l\sigma} + \sum_{lj\sigma} T_{lj}^X d_{l\sigma}^\dagger d_{j\sigma} + U^X \sum_l n_{l\uparrow} n_{l\downarrow} + \sum_{j\sigma} \varepsilon_0^{\mathrm{Fe}} d_{j\sigma}^\dagger d_{j\sigma} + \sum_{jj'\sigma} T_{jj'}^{\mathrm{FeFe}} d_{j\sigma}^\dagger d_{j'\sigma} + U^{\mathrm{Fe}} \sum_j n_{j\uparrow} n_{j\downarrow} + \sum_{lj\sigma} T^{X\mathrm{Fe}} (d_{l\sigma}^\dagger d_{j\sigma} + d_{j\sigma}^\dagger d_{l\sigma}) - J_{df} \sum_l s_l^d \cdot S_l^f, \quad (1)$$

where all the symbols have their usual meanings. We use the functional integral technique [4,5] to treat the d–d electron–electron interaction [3,6]. In this framework of the functional integral method, the initial Hamiltonian with Coulomb correlations is mapped into an effective one-body Hamiltonian in which the electrons are under the action of

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0921-4526/$ - see front matter © 2007 Published by Elsevier B.V.
doi:10.1016/j.physb.2007.10.364

fluctuating charge (v) and spin (ξ) fields. These fluctuating fields which are randomly distributed all over the sites, define a "disorder problem" in both sublattices. We treat this intrinsic disorder in the coherent potential approximation (CPA) and so one defines effective media Σ_σ^{Fe} and Σ_σ^X to restore the translational invariance of the pure Laves phase host. The self-energies are self consistently determined by a CPA equation [6], and thereby the X sublattice host is completely described at any finite temperature.

We consider that the Ta impurity diluted in the X sublattice, defines a Wolf–Clogston problem in the effective medium at the X sublattice. The local d-density of states per spin direction at the impurity site is given by $\rho_{0\sigma}(\varepsilon) = (-1/\pi)\mathrm{Im}\, G_{00\sigma}^{XX}(z)$, where $G_{00\sigma}^{XX}(z)$ is the local perturbed Green function given by

$$G_{00\sigma}^{XX}(z) = \frac{g_{00\sigma}^{XX}(z)}{1 - g_{00\sigma}^{XX}(z)(\varepsilon_\sigma^{Ta} - \Sigma_\sigma^X(z))} \tag{2}$$

and $g_{00\sigma}^{XX}(z)$ is the host Green function written in terms of the self-energy. The energy ε_σ^{Ta} should be self consistently determined by the Friedel screening condition $\Delta Z = \Delta N_\uparrow^X + \Delta N_\downarrow^X$, where ΔN_σ^X is the change in the occupation number at the X sublattice calculated by [7]

$$\Delta N_\sigma^X = -\frac{1}{\pi}\mathrm{Im}\, \ln[1 - g_{00\sigma}^{XX}(\varepsilon_F)(\varepsilon_\sigma^{Ta} - \Sigma_\sigma^X(\varepsilon_F))]. \tag{3}$$

The electron occupation number at the impurity site ($n_{0\sigma}$) is obtained by integrating the local density of states up to the Fermi level, i.e., $n_{0\sigma} = \int_{-\infty}^{\varepsilon_F} \rho_{0\sigma}(\varepsilon) f(\varepsilon)\, d\varepsilon$, $f(\varepsilon)$ being the Fermi function. The local d-magnetic moment at the Ta impurity is then given by $\tilde{m}_d(0) = \sum_\sigma \sigma n_{0\sigma}$. We also consider the s–p sublattice band to describe hyperfine interactions [8]. The local s–p magnetic moment is obtained by $\tilde{m}_c(0) = -\gamma m_d^X$, where m_d^X is the X sublattice d-magnetization and the parameter γ is of order of 0.1 [8]. The total magnetic hyperfine field at the Ta impurity site, is made up by a conduction electron polarization (CEP) contribution due to the s–p conduction electrons and by a core polarization (CP) due to the d conduction electrons. One has $B_{hf} = A(Z_{imp})\tilde{m}_c(0) + A_{CP}^d \tilde{m}_d(0)$, where $A(Z_{imp})$ is the Fermi–Segrè contact coupling parameter and A_{CP}^d is d-core polarization parameter [9].

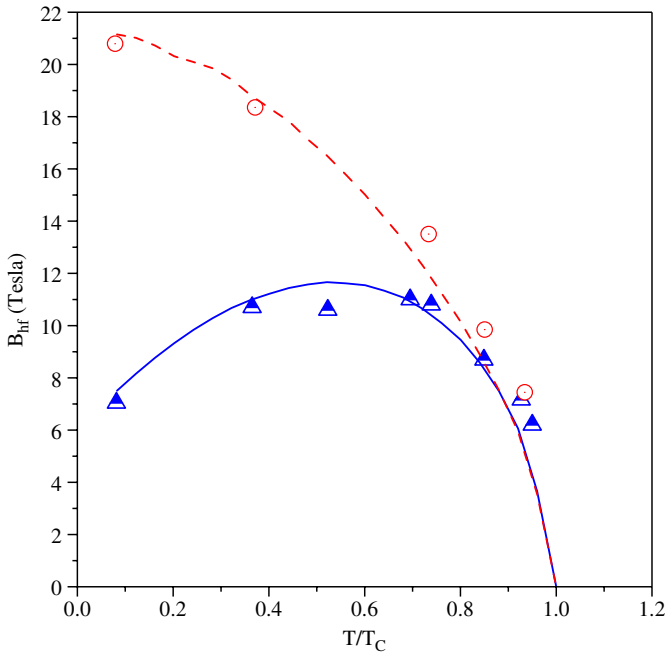

Fig. 1. Magnetic hyperfine field at Ta impurity diluted in $GdFe_2$ intermetallic host. The solid line corresponds to the high pressure calculated total magnetic hyperfine field and the dashed line to the total calculated hyperfine field at normal pressure. Triangles and circles represent experimental data collected from Ref. [2].

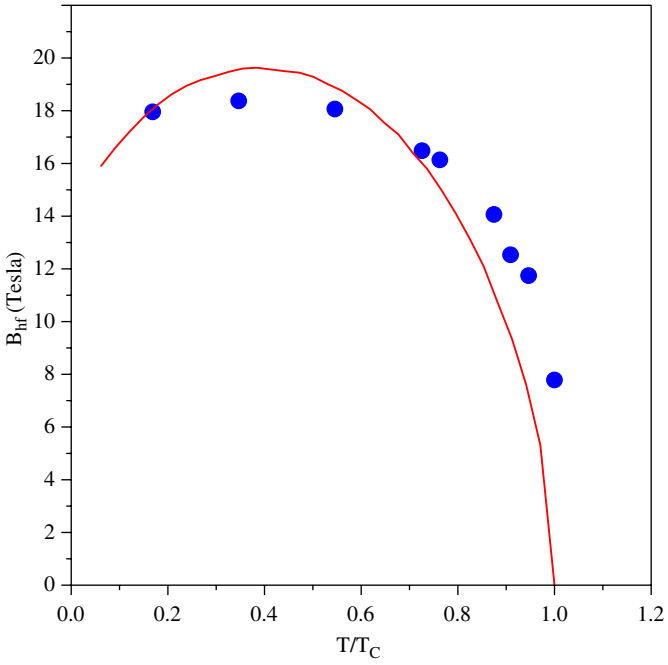

Fig. 2. Magnetic hyperfine field at Ta impurity diluted in $YbFe_2$ intermetallic host. The solid line represents the calculated total hyperfine field and full circles represent experimental data collected from Ref. [11].

In Figs. 1 and 2 we plot as a function of temperature, the calculated magnetic hyperfine field at a Ta impurity dilute in $GdFe_2$ and $YbFe_2$, respectively. Our theoretical calculations exhibit a very good agreement with experiments [1,2], which show that the magnetic hyperfine field at the Ta impurity in $GdFe_2$ and $YbFe_2$ is antiparallel to the magnetization of the Fe sublattice being positive in both cases.

In Fig. 1, we show a semi phenomenological calculation to include pressure effects [10]. In this case, we assume that external pressure excites the elastic degrees of freedom of the host. Therefore one has an electron–phonon interaction which modifies the pure electronic hybridization-like term [12,13], $V_\sigma^X = \varepsilon_\sigma^{Ta} - \Sigma_\sigma^X(\varepsilon_F)$ (see Eq. (3)).

When the electron-phonon interaction is included in Eq. (3), one has a temperature dependence of V_σ^X. Fig. 1 illustrates such pressure effects. The experimental data were obtained for a high pressure of 7.7 GPa and our theoretical results are again in a good agreement with the experimental data reported in Ref. [2].

References

[1] Z.Z. Akselrod, et al., Phys. Stat. Sol. (b) 119 (1983) 667.
[2] O.I. Kochetov, et al., Hyperf. Interact. 59 (1990) 521.
[3] A.L. de Oliveira, N.A. de Oliveira, A. Troper, J. Magn. Magn. Mater. 272 (2004) 631.
[4] R.L. Stratonovich, Dokl. Akad. Nauk. SSSR 115 (1957) 1097.
[5] J. Hubbard, Phys. Rev. Lett. 3 (1959) 77.
[6] N.A. de Oliveira, A.A. Gomes, J. Magn. Magn. Mater. 117 (1992) 175.
[7] A.L. de Oliveira, N.A. de Oliveira, A. Troper, J. Appl. Phys. 91 (2002) 8876.
[8] N.A. de Oliveira, A.A. Gomes, A. Troper, Phys. Rev. B 52 (1995) 9137.
[9] I.A. Campbell, J. Phys. C 2 (1969) 1338.
[10] M.V. Tovar Costa, N.A. de Oliveira, A. Troper, J. Appl. Phys. 81 (1997) 3880.
[11] A.A. Sorokin, et al., J. Exp. Theoret. Phys. 84 (3) (1997) 599.
[12] O.L.T. de Menezes, A. Troper, Phys. Rev. B 22 (1980) 2127.
[13] O.L.T. de Menezes, A. Troper, Physica B 108 (1981) 1345.