ELECTRICAL AND MAGNETIC PROPERTIES

MAGNETIC PROPERTIES OF HCC IRON-NICKEL ALLOYS AT FINITE TEMPERATURES

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Abstract. The dependence of Curie temperature, spin fluctuations, average and local magnetic moments on the concentration of$x$ is investigated for disordered HCC alloy$\mathrm{Fe}_x\mathrm{Ni}_{1-x}$. It is shown how the dependence of the mean and local magnetic moments on concentration varies with temperature. The problem is treated in the renormalized Gaussian approximation of the dynamical theory of spin fluctuations. The numerical results are in good agreement with experiment.

Keywords: *electronic structure, magnetic properties, Slater-Poling curve, spin fluctuations, ferromagnetic alloys*

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1. INTRODUCTION

The analysis of the relationship between the electronic structure and magnetic properties of iron-nickel alloys remains an important problem in theory and applications [1, 2]. A significant part of theoretical works is devoted to the study of the phase diagram (see, e.g., [3, 4]).

In calculations of the magnetic characteristics of HCC iron-nickel alloys at finite temperatures, nonlocal spin correlations are either neglected using the coherent potential approximation and dynamical mean-field theory (PCP+DTSP; see, e.g., [5, 6]) or described using various approximations for effective Hamiltonians with *classical* spins (see, e.g., [7-11]).

Simultaneous consideration of the quantum character and nonlocality of spin fluctuations is realized only in the dynamic theory of spin fluctuations (DTSF) [12]. The use of DTSF allowed us to calculate the temperature dependence of the magnetic characteristics of the invar alloy$\mathrm{Fe}_{0.65}\mathrm{Ni}_{0.35}$ [13, 14] and to obtain the dependence of the Curie temperature of the disordered HCC alloy$\mathrm{Fe}_x\mathrm{Ni}_{1-x}$ on the concentration of$x$ [15].

In the present work, we study in detail the dependence of various magnetic characteristics: spin fluctuations, mean and local magnetic moments - on temperature and concentration$x$ for the disordered HCC alloy $\mathrm{Fe}_x\mathrm{Ni}_{1-x}$. We investigate how the dependence of the mean and local magnetic moments on$x$ changes with increasing temperature (the qualitative nature of these curves in alloys was investigated in [16]), and analyze the similarity of the dependence of magnetic moments and Curie temperature on$x$. The problem is considered in the renormalized Gaussian approximation of dynamic spin fluctuation theory (DTSF-PGA) [12, 14] using spin-polarized densities of electronic states calculated in QCD-PCP [15]. The DTSF-PGA results are compared with other calculations and experiment.

The presentation is organized as follows. Section 2 summarizes the computational scheme. Section 3 gives an overview of the theory and experiment related to the Slater-Poling curve. Section 4 summarizes the results at finite temperatures. In Section 5, conclusions are formulated.

2. THEORETICAL MODEL

The DTSF is based on a quadratic approximation of the free energy $F(V)$ in a fluctuating exchange field V, which allows a self-consistent averaging over all field configurations. At a finite temperature T (in energy units), we solve a system of nonlinear equations for the mean squares of the exchange field fluctuations at the node

$$\langle \Delta V_\alpha^2 \rangle = \frac{1}{N} \sum_{\mathbf{q}} \frac{UT}{2N_\mathrm{d} \lambda_{\mathbf{q}}^\alpha} \frac{2}{\pi} \arctan \frac{U \varphi_{\mathbf{q}}^\alpha \pi^2 T}{6 N_\mathrm{d} \lambda_{\mathbf{q}}^\alpha}, \quad (1)$$

where N is the number of crystal lattice nodes, $N_\mathrm{d} = 5$ is the number of d-bands per atom and spin,

$$\lambda_{\mathbf{q}}^\alpha = 1 - U \chi_{\mathbf{q}}^\alpha(0), \quad \varphi_{\mathbf{q}}^\alpha = \left. \frac{\mathrm{d} \operatorname{Im} \chi_{\mathbf{q}}^\alpha(\varepsilon)}{\mathrm{d}\varepsilon} \right|_{\varepsilon = 0}, \quad \alpha = x, z,$$

for the average exchange field

$$\langle V_z \rangle = -U s_z, \qquad s_z = (n_\uparrow - n_\downarrow)/2, \quad (2)$$

and chemical potential μ

$$n_\mathrm{e} = n_\uparrow + n_\downarrow, \qquad n_\sigma = \frac{1}{\pi} \int \operatorname{Im} g_\sigma(\varepsilon) f(\varepsilon) \mathrm{d}\varepsilon \quad (3)$$

where n_σ is the number of electrons with spin projection $\sigma = \uparrow, \downarrow$ or ± 1, n_e is the total number of electrons (per atom and band). In the given relations $\chi_{\mathbf{q}}^\alpha(\varepsilon)$ is the dynamical susceptibility, $f(\varepsilon) = [\exp((\varepsilon - \mu)/T) + 1]^{-1}$ is the Fermi function,

$$g_\sigma(\varepsilon) = \int \frac{\nu(\varepsilon')}{\varepsilon - \sigma \langle V_z \rangle - \Delta\Sigma_\sigma(\varepsilon) - \varepsilon'} \, \mathrm{d}\varepsilon'$$

- average single-node Green's function, where $\nu(\varepsilon)$ is the non-magnetic density of electronic states (NES) per atom, band and spin, $\Delta\Sigma_\sigma(\varepsilon)$ is the fluctuation contribution to the eigen-energy part calculated by the formula

$$\Delta\Sigma_\sigma(\varepsilon) = \frac{g_\sigma(\varepsilon) \langle \Delta V_z^2 \rangle}{1 + 2\sigma \langle V_z \rangle g_\sigma(\varepsilon)} + 2 g_{\bar{\sigma}}(\varepsilon) \langle \Delta V_x^2 \rangle, \qquad \bar{\sigma} = -\sigma.$$

In the DTSF-PGA, a renormalization of the quadratic approximation of the free energy in the fluctuating field $F(V)$ is made at the expense of high-order terms on V. In the final equations, this leads to renormalization of the mean spin and susceptibility:

$$\tilde{s}_z = (1 + \eta) s_z, \qquad \tilde{\chi}_{\mathbf{q}}^\alpha(\varepsilon) = (1 + 3\eta) \chi_{\mathbf{q}}^\alpha(\varepsilon). \quad (4)$$

The correction factor η is

$$\eta = -\frac{\pi}{W} (2 \chi_\mathrm{L}^x(0) \langle \Delta V_x^2 \rangle + \chi_\mathrm{L}^z(0) \langle \Delta V_z^2 \rangle), \quad (5)$$

where W is the d-band width, $\chi_\mathrm{L}^\alpha(0)$ is the local static susceptibility.

At $T = 0$ the mean squares of fluctuations $\langle \Delta V_\alpha^2 \rangle$ turn to zero and the system transforms into the system of Stoner mean-field theory equations (2) and (3). This makes it possible to find the effective constant U from the known magnetic moment $m_z(T = 0)$, then at $T \neq 0$ the original system is solved by the parameter continuation method with respect to the variables $\langle \Delta V_x^2 \rangle, \langle \Delta V_z^2 \rangle, \langle V_z \rangle, \mu$, and $\Delta\Sigma_\sigma(\varepsilon)$ [17]. The temperature dependence of the magnetic characteristics on the parameters is calculated using the MAGPROP program [18].

The squares of the average $s_z^2 \equiv \langle \mathbf{s} \rangle^2$ and local $s_\mathrm{L}^2 \equiv \langle \mathbf{s}^2 \rangle$ spins differ by the magnitude of the rms spin fluctuation $\Delta s^2 \equiv \langle (\mathbf{s} - \langle \mathbf{s} \rangle)^2 \rangle$:

$$s_\mathrm{L}^2 = s_z^2 + \Delta s^2.$$

(Here $\langle \ldots \rangle$ is the quantum-statistical average at temperature T.) The spin fluctuations are made up of fluctuations at $T = 0$ ("zero") and temperature fluctuations:

$$\Delta s^2 = \Delta s_{\text{zp}}^2 + \Delta s_{\text{temp}}^2.$$

In DTSF we consider only temperature fluctuations, assuming $\Delta s_{\text{zp}}^2 = 0$. We assume that the "zero" fluctuations are already accounted for by renormalizing the constant U . At $T = 0$ the temperature fluctuation also goes to zero: $\Delta s_{\text{temp}}^2 = 0$. Then the average $m_z(T) = gN_{\text{d}}s_z(T)[\mu_{\text{B}}]$ and local $m_{\text{L}}(T) = gs_{\text{L}}(T)[\mu_{\text{B}}]$ magnetic moments at $T = 0$ coincide: $m_z(0) = m_{\text{L}}(0)$. At finite temperature, solving the system of DTSF-PGA equations (1)-(5), we find the local magnetic moment by the formula

$$m_{\text{L}}(T)/m_{\text{L}}(0) = [(\langle V_z(T)\rangle^2 + \langle(\Delta V)^2\rangle)/\langle V_z(0)\rangle^2]^{1/2}.$$

3. MAGNETIC TORQUE AT $T = 0$

The magnetic moment of ferromagnetic metals and alloys at $T = 0$ is fairly well described by Slater's rule, which generalizes Hund's rule for an atom to the case of metals. According to Slater's rule, the magnetic moment (in units of μ_{B}) is equal to the number of spin-uncompensated d-electrons per atom (see [21]). For ferromagnetic metals and alloys we obtain

$$m_z(N_{\text{e}}) = 2N_{\text{d}} - N_{\text{e}}, \qquad (6)$$

where the average number of d-electrons per atom in the metal $N_e = N_{\text{d}}n_{\text{e}}$ can be fractional[1] . The justification of (6) follows from Stoner's theory. From (2) and (3) it follows

$$m_z = N_{\text{d}}(n_\uparrow - n_\downarrow) = 2N_{\text{d}}n_\uparrow - N_{\text{e}}.$$

If the band of d-states with spin up is completely filled (as in Co and Ni), and thus further polarization does not lead to an increase in the magnetic moment, we obtain a linear dependence *decreasing* at an angle of 45 degrees with increasing N_{e} . The maximum magnetic moment is between Fe and Co and corresponds almost entirely to the filled d-band. The dependence of the magnetic moment on the average number of electrons per atom, known as the Slater-Poling curve [19], gives a good approximation for alloys of metals with close atomic numbers, in particular Fe-Co, Co-Ni and Fe-Ni (Fig. 1) .[2]

Fig. 1: Slater-Poling curve for Fe, Co and Ni alloys. Experimental values are taken from [19], except for the HCC alloys Fe-Co [20] and Fe-Ni [4]. The values m_z at $T = 0$, used in the DTSF-PGA calculations, are indicated by asterisks.

The above facts were confirmed by our calculations m_z at $T = 0$ in the Stoner theory [16]. In the framework of Stoner's theory, one can consider that fusion leads only to a shift of the Fermi level [23]. Therefore, the calculations [16] were performed by varying N_{e} for iron, cobalt and nickel PES. However, calculations performed at *finite* temperatures showed that the behavior of the Slater-Poling curve in Stoner theory and in DTSF has even qualitatively different character, due to the fact that Stoner theory completely ignores spin fluctuations.

Fig. 2: PES of d-electrons of disordered HCC alloy $\text{Fe}_x\text{Ni}_{1-x}$ at $0.1 \le x \le 0.6$, smoothed using convolution with the Lorentz half-width function $\Gamma = 0.001\,W$. The vertical dash indicates the Fermi level . ε_{F}

[1] Generalizations of Slater's rule were proposed in [22] (see also [12, Chapter~13]).

[2] As can be seen from Fig. 1, for the Fe-Co and Fe-Ni HCC alloys, branches from the Slater-Poling curve are observed at high iron concentrations.

4. RESULTS AT END TEMPERATURES

We investigate the disordered HCC alloy Fe_xNi_{1-x} at iron concentrations x from 0.1 to 0.6[3], using the same initial non-magnetic PES at $T = 0$, as in [15]. The spin-polarized PES calculated in QCD-PCP for HCC Fe_xNi_{1-x} at x from 0.1 to 0.6 [15] are in good agreement with the spin-polarized PES for $x = 0.4$ and 0.6 calculated in [24]. The non-magnetic PES of the alloy is calculated according to the scheme described in [13]. The obtained PESs are smoothed using convolution with the Lorentz half-width function $\Gamma = 0.001\,W$ to remove unphysical peaks in the zone calculation, which completely ignores the damping of one-electron states. The PESs of the alloys Fe_xNi_{1-x}, normalized to a single d-state (per atom, band and spin), are shown in Fig. 2. The dependence of the magnetic moment at $T = 0$ on the number of electrons lies on the right branch of the Slater-Poling curve corresponding to alloys with HCC lattice (Fig. 1).

Magnetic moment m_z/m_z^0 (calculation – – – – – –, experiment ∘∘∘ [25]), rms fluctuations ($\langle\Delta V_x^2\rangle$ – – – · · – – –) and $\langle\Delta V_z^2\rangle$ (– – – –) in units of mean field square $\bar{V}_z^2$ at $T = 0$, local magnetic moment m_L/m_z^0 (·····) and inverse paramagnetic susceptibility χ^{-1} (– – – · – – –) in units $k_B T_C^{exp}/\mu_B^2$ of disordered HCC alloy Fe_xNi_{1-x} at iron concentrations $0.1 \le x \le 0.6$, calculated in DTSF-PGA as functions of relative temperature T/T_C^{exp}.

The results of calculations of magnetic characteristics in DTSF-PGA are shown in Fig. 4. The temperature dependence of the magnetic moment is in good agreement with experiment [25]. The temperature dependence of the other characteristics agrees well with the results of calculations given in [12] for pure Fe, Co, and Ni. Thus, longitudinal spin fluctuations $\langle\Delta V_z^2\rangle$ predominate in HCC Fe_xNi_{1-x} at concentrations $x = 0.1$ - 0.3, as in pure Ni. Longitudinal $\langle\Delta V_z^2\rangle$ and transverse $\langle\Delta V_x^2\rangle$ spin fluctuations are approximately the same at concentrations $x = 0.4$ -0.5, as in pure Co. Finally, the transverse $\langle\Delta V_x^2\rangle$ spin fluctuations predominate at concentrations $x = 0.6$, as in pure Fe. Similarly, the local moment m_L increases with temperature at $x = 0.1$ -0.3, as in Ni, is nearly constant at $x = 0.4$, as in Co, and decreases with temperature at $x = 0.5$ -0.6, as in Fe. The homogeneous paramagnetic susceptibility $\chi^0(0)$ satisfies the Curie-Weiss law at all x, as for pure metals.

The dependence of Curie temperature on nickel concentration is shown in Fig. 3. The experimental curve has a maximum near 70 at.% Ni. The curve in DTSF-PGA is in good agreement with the experimental curve [3, 26]. The results of local approximations: static PCP approximation [27] and dynamic PCP+DTSP approximation [6] are presented for comparison. As can be seen, in the static [27] the maximum T_C is noticeably shifted towards bo′ lier concentrations of Ni[4]. The calculation in the single-node dynamic PCP+DTSP approximation [6] leads to significant differences from the static results [27].

Fig. 3: Curie temperature dependence T_C for disordered HCC alloy Fe_xNi_{1-x} on nickel concentration $1 - x$ at $0.1 \le x \le 0.6$, calculated in the dynamic nonlocal DTSF-PGA theory, in one-hole theories: static PCP approximation [27] and dynamic PCP+DTSP approximation [6] - and in experiment [3, 26].

[3] At iron concentrations $x > 0.7$ HCC alloy Fe_xNi_{1-x} becomes antiferromagnetic.

[4] In [28], an attempt was made to go beyond the one-node approximation in statics [27], but it did not yield noticeable differences for Fe-Ni alloys.

The results obtained using various approximations for the effective Hamiltonians with classical spins [9, 10, 15] give good quantitative agreement with experiment at some concentrations, but do not give the correct course of the temperature dependence of T_C on concentration in general. In particular, the maximum of T_C in the calculations [9, 10, 15] is noticeably shifted toward small Ni concentrations, contrary to experiment (Fig. 3).

The dependence of the Curie temperature T_C on the average number of electrons per atom for Fe, Co and Ni alloys is shown in Fig. 4. This dependence has some similarity with the Slater-Poling curve (Fig. 1). However, the differences in the behavior of T_C for HCC Fe-Ni and Co-Ni alloys (as well as for OCC Fe-Ni and Co-Ni alloys) are much more noticeable than in the behavior of m_z at $T = 0$. In addition, for the disordered HCC alloy Fe_xNi_{1-x} , the maximum of the Curie temperature T_C is reached at bo′ higher nickel concentrations than the maximum of the m_z dependence at $T = 0$ on the Slater-Poling curve.

The curves of the average magnetic moment m_z , as a function of nickel concentration at finite temperatures, are shown in Fig. 5. As can be seen, with increasing temperature, the Slater-Poling curve shifts to zero.

Fig. 4: Dependence of Curie temperature T_C on the average number of electrons per atom for Fe, Co and Ni alloys. The experimental values are taken from [26], except for the HCC alloys Fe-Co [29] and Fe-Ni [4]. The values T_C , calculated in DTSF-PGA, are indicated by asterisks.

The dependence of m_z on Ni concentration at room temperatures remains practically a straight line parallel to the Slater-Poling curve, in full agreement with the experiment [30]. With further temperature increase, the dependence of the magnetic moment m_z on concentration becomes curved and becomes similar to the Curie temperature dependence T_C on concentration (Fig. 3). The maximum of m_z is gradually shifted towards bo′ higher Ni concentrations and at high temperatures is between 50 at.% and 60 at.% Ni. These results are in qualitative agreement with the results of DTSF calculations, which were obtained by varying the number of d-electrons for iron, cobalt and nickel PES in our work [16].

The dependences of the local magnetic moment as a function of nickel concentration at different temperatures are shown in Fig. 6 (temperatures are the same as in Fig. 5). As can be seen, the linear dependence of the local magnetic moment on concentration changes weakly with increasing temperature up to room temperature. With further temperature increase, the decreasing dependence remains, but the scatter of the local moment values gradually decreases. Extrapolation of our results at T_C is in reasonable agreement with the experimental values m_L , obtained in neutron scattering: 1.55-1.7 for Fe and 0.6-0.9 for Ni (for details see [12, 31] and references there). The appearance of the dependence of the local moment on concentration is fundamentally different from the dependences of the Curie temperature and the mean magnetic moment on concentration (Figs. 3 and 5). In particular, the maximum m_L is reached at the concentration of nickel $1 - x = 0.4$ at all temperatures, except for temperatures near $T = 600$ K, where it shifts slightly toward bo′ higher nickel concentrations: $.1 - x = 0.5$

The qualitative course of the local momentum-concentration dependence at high temperatures was correctly predicted in our DTSF calculations [16]. However, for the real alloy, the curves at high temperatures turned out to be more convex upward (Fig. 6) than predicted by our preliminary analysis.

Fig. 5: Dependence of average magnetic moment m_z for disordered HCC alloy Fe_xNi_{1-x} on nickel concentration $1 - x$ at $0.1 \leq x \leq 0.6$, calculated in DTSF-PGA at different temperatures.

5. CONCLUSION

Simultaneous consideration of the quantum and non-local character of spin fluctuations in DTSF-PGA allowed us to calculate the dependences of average and local magnetic moments, spin fluctuations and paramagnetic susceptibility on temperature for disordered HCC alloyFe_xNi_{1-x} at $.0.1 \leq x \leq 0.6$

The temperature dependence of the magnetic moment is in good agreement with experiment. Longitudinal spin fluctuations dominate at concentrations$x = 0.1$ -0.3 (as in pure Ni), longitudinal and transverse fluctuations approximately coincide at concentrations$x = 0.4$ -0.5 (as in Co) and finally transverse fluctuations dominate at concentrations$x = 0.6$ (as in Fe).

The dependence of the average magnetic moment on concentration remains practically a straight line parallel to the Slater-Poling curve up to room temperature, in full agreement with the experiment. With further temperature increase, the dependence of the magnetic moment on concentration becomes curved and becomes similar to the Curie temperature dependence on concentration: it has a pronounced maximum between 50 at.% and 60 at.% Ni.

The dependence of the local magnetic moment on concentration also remains almost linear up to room temperatures. However, this straight line is not parallel to the Slater-Poling curve, and its slope decreases with increasing temperature. With further temperature increase, the dependence of the local magnetic moment on concentration remains decreasing, but becomes nonlinear. The maximum of the local moment is reached at concentrations of 40 at.% and 50 at.% Ni.

A detailed study of the *paramagnetic* properties of HCC iron-nickel alloys in DTSF-PGA is the task of our further investigation.

Fig. 6: Dependence of local magnetic momentm_{L} for disordered HCC alloyFe_xNi_{1-x} on nickel concentration$1 - x$ at$0.1 \leq x \leq 0.6$, calculated in DTSF-PGA at different temperatures. The inset shows larger values at nickel concentrations$1 - x = 0.7$ and $.1 - x = 0.8$

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CONFLICT OF INTERESTS

The authors declare that they have no conflict of interest.

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