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Magnetic properties of Fe–Al for quenched diluted spin-1 Ising model

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ABSTRACT

We study the phase diagram of $Fe_{1-q}Al_q$ alloys via the quenched site diluted spin-1 ferromagnetic Ising model by employing effective field theory. One suggests a new approach to exchange interaction between nearest neighbors of Fe that depends on the powers of the Al (q) instead of the linear dependence proposed in other papers. In such model we propose the same kind of the exchange interaction in which the iron–nickel alloys obtain an excellent theoretical description of the experimental data of the T–q phase diagram for all Al concentration q.

1. Introduction

In the last years, the Fe–Al alloys have obtained the interest of many researchers as they exhibit several hightech properties, such as resistance to oxidation and corrosion, good ductility at room temperature, relatively low density, high value of magnetic permeability as well as vibration damping and insulating properties. On the other hand, Fe–Al alloys have been of particular interest because it is possible to induce novel kinds of critical behavior [2,19,26] including different types of phase transitions, such as the ferromagnetism, paramagnetism and the re-entrant spin-glass phase [3,7,21,24]. In contrast to theoretical predictions, there is a slight variation in the critical temperature at low concentration of Al atoms ($q<0.2$) and spin models used in the literature so far have not considered the effective Fe spin atom [2,10].

The disordered $Fe_{1-q}Al_q$ alloys are arranged in a bcc lattice structure, and each site is randomly occupied by atoms of Fe or Al [10,12,27]. When the Al concentration increases, for $q>0.2$ the transition temperature from ferromagnetic to paramagnetic phase decreases and vanishes in the vicinity of $q=0.7$ [27]. For $q<0.3$, $T_c(q)$ has anomalous behavior which is not explained so far by theoretical models contained in the literature [2,10,20]. The proposals recently employed concern the use of a superexchange interaction (see Refs. [10,20] and references therein) to explain this anomalous behavior. However, this approach has no experimental support [5,27].

In this work, we study the quenched diluted spin-1 Ising model for Fe–Al alloys, with a probability distribution function of the exchange couplings for cluster containing one spin on a bcc lattice. The calculation is carried out within the effective field theory (EFT) approximation.

2. Model and formalism

The Hamiltonian considered is given by

$$\mathcal{H} = -J(q)\sum_{\langle i,j\rangle}\epsilon_i\epsilon_j S_i^z S_j^z, \tag{1}$$

where the summation is performed over all pairs of the nearest-neighboring sites $\langle i,j\rangle$. The quantities S_i^z are isotropically interacting classical spins localized at the sites i of a bcc lattice, $J(q)$ is the exchange coupling between the spins, ϵ_i takes values 1 or 0 and it obeys the following probability distribution:

$$P(\epsilon_i) = p\delta(\epsilon_i - 1) + q\delta(\epsilon_i), \tag{2}$$

where p and q are the concentrations of Fe and Al atoms, respectively, and $p+q=1$.

In the present work, our results are based on the extension of results obtained in previous works [12,13]. By employing the EFT with differential operator technique, the average magnetization per spin is given by

$$\langle S_i^z\rangle = \left\langle \prod_j e^{\beta J(q)\epsilon_i\epsilon_j S_j^z D_x}\right\rangle f(x)|_{x=0}, \tag{3}$$

where $D_x \equiv \partial/\partial x$ and

$$f(x) = \frac{2\sinh(x)}{2\cosh(x)+1}. \tag{4}$$

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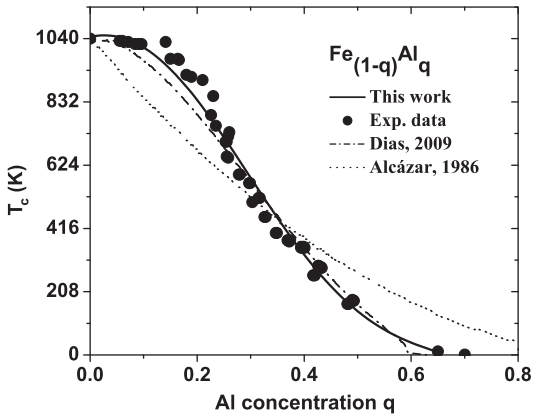

Fig. 1. Phase diagram in the T–q plane for $Fe_{1-q}Al_q$. The solid line is a fit as described in the text. Dotted line is the previous fit using the Bogoliubov procedure [2] and the dashed line is the result assuming superexchange interactions between next nearest-neighbors [10]. Solid circles are the experimental data [27].

By employing the generalized van der Waerden identity [4,25] for spin $S=1$, one gets

$$\langle S_i^z\rangle = \langle [1+S_j\sinh(K_{ij}D_x)+S_j^2(\cosh(K_{ij}D_x)-1)]^Z\rangle f(x)|_{x=0}, \tag{5}$$

where Z is the coordination number ($Z=8$ for bcc lattice), $K_{ij}\equiv\beta\epsilon_i\epsilon_j J(q)$. Here, we will focus our attention on the second-order transition line. Then, by performing the configurational averaging in Eq. (5) (here, denoted by $m_z=\langle\langle S_i^z\rangle\rangle_c$) and by expanding up to first order in this parameter, we obtain

$$m_z = A_1(q,K)m_z + \mathcal{O}(m_z^3), \tag{6}$$

with

$$A_1(q,K) = 8(1-q)^2\sinh(KD_x)f(x)|_{x=0}, \tag{7}$$

where the coefficient $A_1(q,K)$ can be easily calculated by applying the mathematical relation [8]

$$2\sinh(aD_x)f(x) = f(x+a)-f(x-a).$$

3. Results and remarks

It is observed that the substitution of Fe by Al atoms produces a lattice expansion for the diluted Fe–Al alloys. This variation in the lattice parameter is attributed to the larger atomic size of the Al atom [27]. This phenomenon has been also highlighted by others several authors [1,2,5,27]. On the other hand, the diluted $Fe_{1-q}Al_q$ produces a reduction in the exchange coupling. Based on the work by Kaul [17], Alcazar and da Silva [1] have considered both a linear dependence of lattice parameter r and that of the exchange coupling J, on the composition q (See Refs. [11,12,13]). Unlike, in the present work, we consider that the relationship between J and q has the form

$$J(q) = J_0 e^{(Aq+Bq^2+Cq^3)}, \tag{8}$$

where A, B and C are theoretical parameters to be fitted to the experimental data. By following the same ideas of References [11,12,13], with $J_0=17.0$ meV and by adjusting the experimental data for the lattice parameter r versus q for the $Fe_{1-q}Al_q$ alloys [27], one gets $A=2.38$, $B=-5.60$ and $C=-2.3$. Taking an exchange interaction in terms of expansion of quadratic and cubic powers of q corrects the theoretical prediction without the need for introduction of the superexchange interaction [12,13]. We can justify the functional dependence of the exchange integral $J(q)$ on distance r by assuming the same behavior of exchange interaction as in iron–nickel alloys (see Refs. [11,12,13,15,17,18] and references therein). On the other hand, there is an experimental evidence of the nonlinear dependence of r with q, namely the amorphous alloys [17]. In Refs. [11,12] there is a fit proposed for the $r(q)$ curve in terms of powers of q for the site-diluted spin-1/2 Ising model, but the $T_c(q)$ curve vanishes in $q_c\approx 0.54$, very below the experimental value obtained for $Fe_{1-q}Al_q$ alloys, $q_c=0.7$ [27].

In the vicinity of the second-order phase, $m_z\simeq 0$, since the magnetization m_z goes to zero continuously, then

$$A_1(q,K) = 1, \tag{9}$$

provides the second-order transition line [9,16].

A good fit to the experimental data [27] is obtained considering a numerical treatment, which can be accomplished without great difficulty and Eq. (9) provides the critical parameters K_c^{-1} and q_c for the system under consideration. As can be seen in Fig. 1, our results show an excellent agreement with the experimental data for q values varying from 0 to 0.754. On the other hand, $T_c=K_c^{-1}=1040$ K (for $q=0$) and the critical concentration is $q_c=0.647$. The result obtained in the literature for bcc lattice is $q_c=0.754$ according to Refs. [6,22,23]. At this point, it is worthwhile to mention that in our previous work, Freitas et al. (2013) [14], by employing the quenched diluted high-spin $S=2$ Ising model and by using similar approximate framework, we also obtain a very reasonable theoretical description of the experimental data for the behavior in the $T-q$ phase diagram for the Fe-Al alloys. It predicts, however, a much higher value for the Fe-Al alloys. It predicts, however, a much higher value for the critical concentration $q_c (i. e., $q_c = 0.77$). Here, on the other hand, the present calculation provides a much better fit for the transition temperature curve (i. e. $T_c(q)$) to the experimental data for all region of Al concentration q, given in particular, the observed experimental value for the critical concentration $q_c=0.647$ (Yelsukov et al. [27]), revealing the best agreement between theory and experiment published so far in the literature.

In contrast to Refs. [2,10,20], our results demonstrate a very good agreement also for $q<0.2$, the region known as anomalous. Dias et al. and Plascak et al. [10,20] have obtained reasonable agreement with the experimental data using antiferromagnetic super-exchange interaction. However, there is no experimental evidence to ensure that hypothesis.

The applicability of the one-spin cluster EFT scheme for spin-1 Ising model with nonlinear exchange coupling provides a good description for the behavior of the T–q phase diagram for the Fe–Al alloys. On the other hand, previous works in the literature have not obtained a good agreement between theory and experiment. Finally, we observe that our approach can be easily extended for the description of magnetic properties and, also, the extension for cluster with $N\geq 2$ spins which will be the aim of future study.

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