Mean field renormalization group: A theoretical approach to the $Fe_{1-q}Al_q$ in the bcc lattice

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In this work, the site diluted Heisenberg model is applied to study the magnetic properties of the bcc disordered phase of FeAl alloys by employing mean field renormalization group theory. We suggest a new approach to exchange interaction between nearest neighbors of Fe that depends on de powers of the Al (q) instead of the linear dependence proposed in other papers. Excellent agreement with the experimental data in the $T - q$ plane have been obtained, in particular, in the region with anomalous behavior of the alloy concerned. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4729001]

I. INTRODUCTION

In recent years, the pure and disordered magnetic systems have been a source of active research, highlighting the potential for technological applications and also of relevant importance as a prototype for theoretical and experimental studies.[1–5] In this context, many disordered magnetic systems have been of a particular interest because it is possible to induce novel kinds of critical behavior, e.g., one can mention the FeAl alloy for the study of theoretical models involving phase transitions. The FeAl alloy has drawn the attention of many researchers due to promising high-tech properties such as resistance to oxidation and corrosion, good ductility at room temperature, relatively low density, magnetic permeability as well as vibration damping and insulating properties.[6,7] The resistivity of FeAl alloys is proportional to the concentration of Al. However, the saturation magnetic induction is decreased by the increase of Al atoms.

In the disordered phase, the FeAl alloy is arranged in a bcc lattice structure and each site is randomly occupied by atoms of Fe or Al. When the Al concentration increases, the transition temperature from ferromagnetic to paramagnetic phase decreases and vanishes in the vicinity of $q = 0.54$. This variation in temperature with the concentration of Al atoms exhibits an anomalous behavior in the region of $q < 0.3$, which is not explained by other theoretical models. On the other hand, there are proposals of the existence of anti-ferromagnetic superexchange interaction, which are not supported by experimental studies.[7,8]

Information about the behavior of pure or disordered magnetic systems at the phase transition has been gathered by several experimental and theoretical studies.[9–12] In the former case, many theoretical problems associated with such systems have been studied extensively by many authors, some analytical approaches, as well as computationally exact approximations (Monte Carlo simulations, as example), have been developed in order to treat such systems. Among these approaches is the mean field theory (MFT).[13,14]

The MFT technique has been applied to the study of critical phenomena in classical and quantum spin models that display first- and second-order phase transitions and tricritical points in phase diagram and has provided useful qualitative and quantitative insights into critical behavior of these systems.[15–21]

In the last years, various approximations within the real-space renormalization group methods have been developed to study the critical behavior of pure and random diluted spin systems.[22,23] In particular, studies on some models have been performed by employing the mean field renormalization group (MFRG)[13,14] and effective field renormalization group (EFRG)[4,24] methods.

In the RG scheme, such as, the MFRG (Refs. 13, 14, and 25) method has been successfully employed in spin systems, where the results obtained are in accordance with other more effective approach (series expansion, Monte Carlo simulation among others). The approaches are based on comparison of two clusters of different sizes, each of them simulating infinite systems.

In this work, we used the MFRG scheme in an site-diluted Heisenberg model to study the behavior of $Fe_{1-q}Al_q$, with particular attention to the anomalous region of the phase diagram in the $T - q$ plane for cluster containing one spin on a bcc lattice and only interactions between nearest neighbors are considered. We consider an exchange interaction, J, in terms of an expansion up to third power of q. This approach differs from earlier works in literature and leads to a good agreement with the experimental data.

The outline of the remainder of the work is as follows: in Sec. II, the model and formulations are introduced. In Sec. III, results and discussions are presented and in Sec. IV, the final results are highlighted.

II. MODEL AND CALCULATIONS

The considered Hamiltonian for this model is given by

$$\mathcal{H} = -\sum_{(ij)} J\epsilon_i\epsilon_j[S_i^z S_j^z + \eta(S_i^x S_j^x + S_i^y S_j^y)], \qquad (1)$$

where the summation is carried out only over pairs of nearest-neighboring sites (i,j), the quantities $S_i^\nu(\nu = x, y, z)$

are the Pauli matrices at the sites i of a bcc lattice and η is the anisotropy parameter. The Hamiltonian given by Eq. (1) reduces to the well-known isotropic Heisenberg and Ising models for $\eta = 1$ and 0, respectively. $J > 0$ is the exchange interaction between the spins and $\epsilon_i = 0$ or 1 depending if site is occupied by Al or Fe atom, which is assumed to be randomly distributed according to the probability distribution function,

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

where p is the concentration of Fe atoms and q of the Al atoms, obeying the relation $p + q = 1$.

In the present work, we follow the same ideas of a procedure previously developed in Ref. 26 to obtain the average magnetization per spin for one and two-spin, respectively. Based on this approximation, b' and b simulate the effect of surrounding spins in the infinity system. So, b' and b are the symmetry breaking fields. On the other hand, considering that for such random system, it is necessary to perform the random average in the equation for magnetization per spin, $\langle S_i^z \rangle_c$, then

$$m_1 = \langle S_1^z \rangle_c = K' p'^2 b' Z, \tag{3a}$$

$$m_2 = \langle S_2^z \rangle_c = Kbp^2(Z-1)\left[\frac{2p}{1 + e^{-2K}\cosh(2\eta K)} + q\right]. \tag{3b}$$

Here, Z denotes the coordination number. Following the ideas of Indekeu, Maritan, and Stella,[13] using m_1 and m_2, in Eq. (3a) and noticing that in the vicinity of the critical temperature $b'(b) \to 0$, we find the transition critical line,

$$K' = K\left(\frac{Z-1}{Z}\right)\left[\frac{2p}{1 + e^{-2K}\cosh(2\eta K)} + q\right], \tag{4}$$

where we impose $p' = p$. Equation (4) gives a recursion relation involving the coupling constants; i.e., $K' = K'(K)$, where in the fixed point $K^\star$ we have $K' = K = K^\star$. In the case a nontrivial fixed point we obtain the critical coupling K_c system by solving the fixed-point equation $K^\star = K(K^\star)$ when the symmetry-breaking occurs.

III. RESULTS AND DISCUSSIONS

The variation of the bcc lattice parameter $r(q)$ versus the aluminum concentration q, reported by several authors[27–29] is shown in Figure 1. It is noted that the substitution of Fe by Al atoms produces a lattice expansion, and this variation in the lattice parameter is attributed to the larger atomic size of the Al atom. Up to now, it has been assumed in Ref. 27 that the lattice parameter r of the $Fe_{1-q}Al_q$ alloys depends linearly on the composition q.

However, looking closely at Figure 1, a deviation is observed between the experimental data and linear model, especially for the $q > 0.25$ concentrations. Thus, the data can be best least-squares fitted with a slight cubic dependence as

$$r(q) = a_0 + a_1 q + a_2 q^2 + a_3 q^3, \tag{5}$$

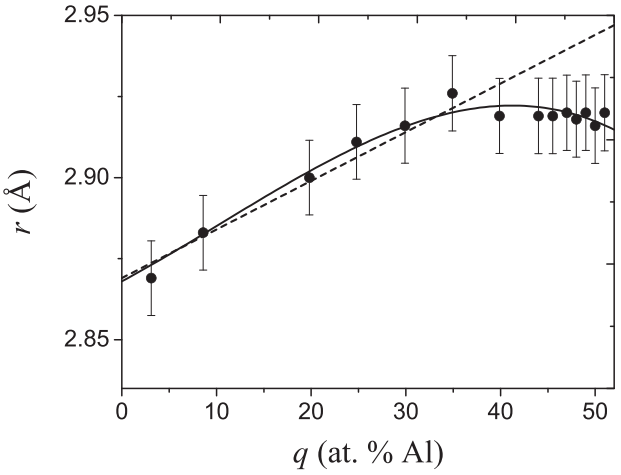

FIG. 1. The lattice parameter of disordered FeAl alloys as a function of Al concentration. The full line is the fit to Eq. (5), and the dashed straight line corresponds to fit used in Ref. 27, dots are the experimental data.[30]

where $a_0 = 2.866$ Å, $a_1 = 0.252$ Å, $a_2 = -0.164$ Å, and $a_3 = -0.230$ Å.

The dilution of the iron with aluminum atoms produces a reduction in the exchange interaction. In first approximation, Alcazar *et al.*[30] considered that the lattice constant r, dependence of the exchange interaction J_1, is linear. Therefore, we suggest that the relationship between J_1 and q has the form,

$$J_1(q) = J(1 + Aq + Bq^2 + Cq^3), \tag{6}$$

where A, B, and C are theoretical parameters to be fitted to experimental data.[30] Using $J = 12.7$ meV and applying a careful adjustment to the experimental data, one gets $A = 1.65, B = -4.90$, and $C = -0.35$ (see Sec. III). The quadratic and cubic terms correct the theoretical prediction without the need for introduction of the superexchange interaction.[7]

At this point, we will consider a numerical treatment which can be done without great difficulty. Thus, we carry out numerical calculations to show results which show a remarkable improvement that has been previously reported in the literature. The recursion relation (4) yields the critical parameters K_c^{-1} and q_c of the system for the model under consideration in this work. The critical frontiers associated to the site-diluted Heisenberg model are presented in Fig. 2 for a bcc lattice and, in particular, we compare our results with the experimental data.[7,28,29,31] In contrast to other works in the literature[26,30,31] (and references therein), the phase diagram shows that our results are in excellent agreement with experimental data for all ranges of q, with emphasis on the anomalous region ($q < 0.2$). In general, the theoretical models that have been used to study the behavior of the FeAl alloy show only slight agreement with the results obtained for the region $q > 0.3$.[26,31] On the other hand, the simple cubic dependence on q for J_1, and the obtained results suggest that there is no need of dependence with a superexchange interaction as proposed by the authors Dias

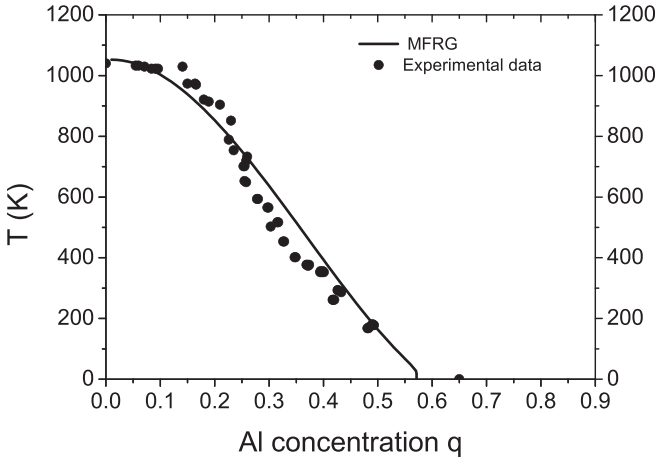

FIG. 2. Magnetic transition temperature as a function of Al concentration in according to our model (black line). Dots are the experimental data.

et al.,[31] as well as describing J_1 in terms of constants that are not physically acceptable.

For small values of q ($q < 0.2$), the phase transition temperature of FeAl approaches the value obtained for the Fe atom ($T_C = 1040\,\mathrm{K}$).[7] On the other hand, the increased concentration of Al atoms below $q \simeq 4/7$ the system remains magnetically ordered and the transition temperature decreases continuously. The dependence of the magnetic transition temperature, T_C on the Al concentration q in alloys is seen to be essentially nonlinear. We observe that for the experimental data slightly above $q = 0.2$ there is a sharp drop in the transition temperature. Some of the attempts to explain this behavior led to the proposition of antiferromagnetic superexchange interactions in the range below $q = 0.3$. However, there is no experimental evidence to support such a proposition.

The agreement between theoretical prediction and experiment is very good, even in the anomalous range, $0.2 < q \lesssim 0.3$. Now, for $q > 0.3$, there is a relatively decrease in transition temperature as a function of q. The value achieved for the reduced critical temperature was the same as that obtained by Dias *et al.*[7]: $k_B T_C/J_1 = 7.0606$.

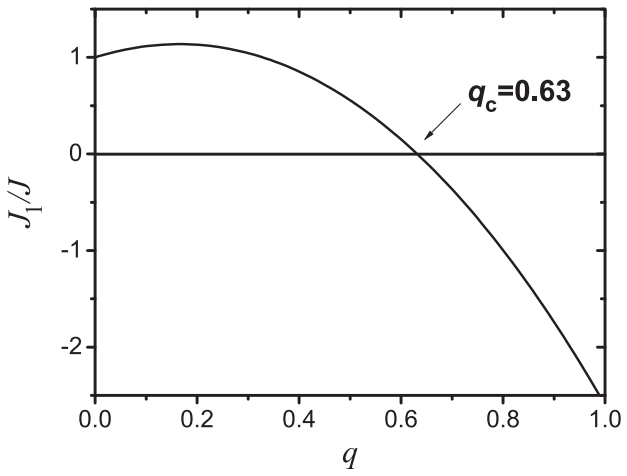

FIG. 3. Normalized exchange interaction as a function of the Al concentration.

We can highlight a few features of the graph of $J_1(q)$ shown in Figure 3, the object of our proposition to the Eq. (6). It is noticed that in the range $0 < q \leq 0.165$, $J_1(q)$ increases until a maximum of $J_1(q^\star = 0.165) = 14.443$ eV. For $q > q^\star$, $J_1(q)$ decreases to cancel up to critical temperature $q_c = 0.63$. From $q > 0.63$ to $q = 1$, $J_1(q)$ is negative; however for this range of Al concentration, there is no magnetic ordering for $T > 0$. In fact, the predicted behavior above T_c is meaningless. Here, the $J_1(q)$ is similar to the superexchange interaction introduced in by authors of Ref. 7. This ensures the fact that no need for the introduction of the superexchange interaction, and signals a more general character of $J_1(q)$ used here: for $q > 0.165$, $J_2(q)$ (superexchange interaction) becomes much smaller than $J_1(q)$. In the region $0 < q < 0.3$, we can suggest that the $J_1(q)$ is something like a sum of an exchange interaction linear and a superexchange interaction written in terms of other powers of q.

We wish to emphasize that for high values of the parameter q, the non-magnetic atoms are clustered they destroy much less than bonds when they are separated in the lattice, a fact that explains the decrease of the transition temperature for increasing values of the mixing probability (see Ref. 32 and references therein).

On the other hand, MFT takes the magnetizations of carriers and ion spins to be uniform in space and neglects correlations and long-wavelength collective fluctuations between them. In other words, the effect of the quantum fluctuations that are important in the low-temperature region; mean field approximation is not adequate to approach quantum systems.

IV. CONCLUSIONS

With the advantage of simplicity, the model presented here can solve the problem of describing the anomalous behavior of FeAl alloy in the region of low concentration of Al. The phase diagram (Figure 2) shows a good qualitative and quantitative behavior with experimental data for all ranges of q. The proposed form for the exchange interaction appears as an extension of models previously proposed, and can be used for describing the magnetic behavior of other alloys.

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