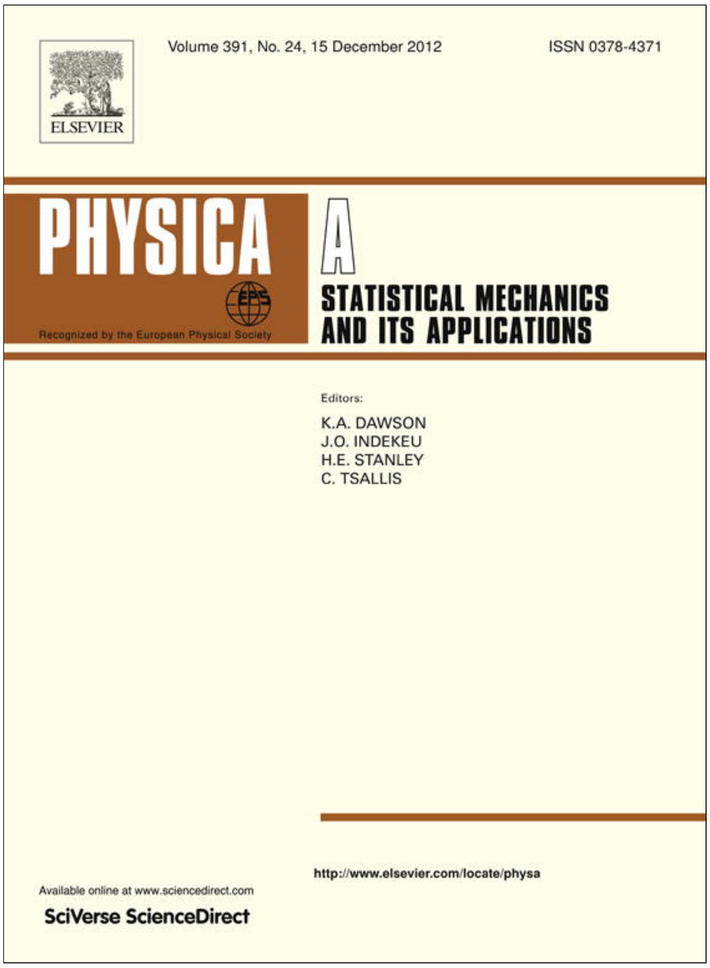
ELSEVIER
Volume 391, No. 24, 15 December 2012
ISSN 0378-4371
PHYSICA A
Recognized by the European Physical Society
STATISTICAL MECHANICS
AND ITS APPLICATIONS
Editors:
K.A. DAWSON
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http://www.elsevier.com/locate/physa
Available online at www.sciencedirect.com
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Physica A 391 (2012) 6332–6336

Contents lists available at SciVerse ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

A new theoretical approach to the $Fe_{1-q}Al_q$ in the bcc lattice by employing effective field theory

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ARTICLE INFO

Article history:
Received 22 March 2012
Received in revised form 18 May 2012
Available online 14 July 2012

Keywords:
FeAl alloys
Effective field
Ising model

ABSTRACT

In this work, a study on a site diluted Ising model system is applied to the magnetic properties of the bcc disordered phase of FeAl alloys by employing effective field theory. Here, 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. With this, we find an excellent agreement for the description of experimental data and the phase diagram in the $T - q$ plane, in particular, the region with anomalous behavior of the alloy concerned.

1. Introduction

In recent years, pure and disordered magnetic systems have been a source of active research, highlighting the potential for technological applications and also their relevant importance as prototypes for theoretical and experimental studies [1–5]. In this context, many disordered magnetic systems have been of 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 an 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 the 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 latter 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 an example), have been developed in order to treat such systems. Among these approaches, and beyond mean field theory, [13,14] is the effective field theory [15,16] based on the Callen–Suzuki relation [17,18].

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0378-4371/$ – see front matter
doi:10.1016/j.physa.2012.06.068

The effective field theory (EFT) technique has been applied to the study of critical phenomena in classical and quantum spin models (e.g., the transverse Ising model, Blume–Capel model, the ferromagnetic and antiferromagnetic Heisenberg quantum model, the Heisenberg frustrated model and others) that display first-and second-order phase transitions and tricritical points in the phase diagram and has provided useful qualitative and quantitative insights into critical behavior of these systems [4,16,19]. The results are achieved by treating the effects of the surrounding spins of each of the clusters through a convenient differential operator expansion technique introduced in the literature by Honmura and Kaneyoshi [20], taking all relevant self-spin correlations into account and including the contribution of the set of spins.

In this work, we used the EFT technique in an Ising model of spin-1/2 to study the behavior of $Fe_{1-q}Al_q$, with particular attention on the anomalous region of the phase diagram in the $T-q$ plane for a cluster containing one spin on a bcc lattice and only interactions between nearest neighbors being 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 the literature and leads to a good agreement with the experimental data.

The outline of the remainder of the work is as follows: in Section 2, the model and formulations are introduced. In Section 3, results are presented.

2. Model and calculations

The considered Hamiltonian for a site-diluted Ising model is given by

$$\mathcal{H} = -J_1 \sum_{(i,j)} \epsilon_i \epsilon_j \sigma_i \sigma_j, \tag{1}$$

where the summation is carried out only over pairs of nearest-neighboring sites (i, j), the quantities $\sigma_i = \pm 1$ at the sites i of a bcc lattice. J_1 is the exchange interaction between the spins and $\epsilon_i = 0$ or 1 depending whether the site is occupied by Al or Fe atoms, which are 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 and q are the concentrations of Fe atoms and Al atoms, respectively, obeying the relation $p + q = 1$.

In the present work, we follow the same ideas as a procedure previously developed in Refs. [4,16,21]. In order to obtain the average magnetization per spin for a one-spin cluster, we use the exact Callen's relation [17] to obtain

$$m = \left\langle \tanh\left(\sum_{(i,j)} \beta J_{ij} \sigma_j\right)\right\rangle, \tag{3}$$

where $J_{ij} = J_1 \epsilon_i \epsilon_j \, (\equiv K_{ij} = \beta J_{ij}, \ \beta = 1/k_B T)$. According to the properties of the differential operator [20] the average magnetization is given by

$$m = \left\langle \prod_j e^{\beta J_{ij} \sigma_j D_x} \right\rangle \tanh(x)\Big|_{x=0}. \tag{4}$$

Eqs. (3) and (4) are exact and applied here as the basis of our formalism, since it yields the cluster magnetization and the corresponding multi-spin correlation functions associated with various sites for the cluster under consideration. By using the van der Waerden identity [22] [i.e., $\exp(\sigma_i \zeta) = \cosh(\zeta) + \sigma_i \sinh(\zeta)\,;\ \forall\, \zeta$], one gets

$$m = \left\langle \prod_j \left[\cosh(K_{ij} D_x) + \sigma_j \sinh(K_{ij} D_x)\right] \right\rangle \tanh(x)\Big|_{x=0}. \tag{5}$$

For such a system, it is necessary to perform the thermal and random average in Eq. (5). In other words,

$$\bar{m} = \sum_{l=0}^{s} A_{2l+1}(q, K) \bar{m}^{2l+1}, \tag{6}$$

where $\bar{m}$ means the configurational average of m and the coefficients $A_{2l+1}(q, K)$ may be determined by using the properties of the differential operator.

In this work, we are interested in the phase boundary of the model under consideration. Then we focus our attention in the second-order transition line, where only the Ising case is studied. In the vicinity of the second-order phase transition $\bar{m} \simeq 0$, then Eq. (6) can be rewritten as

$$\bar{m}^2 = -\frac{A_1(q, K) - 1}{A_3(q, K)}. \tag{7}$$

Since the magnetization $\bar{m}$ goes to zero continuously, a second-order transition line is obtained from simultaneous solution of the equations

$$A_1(q, K) = 1, \qquad A_3(q, K) < 0. \tag{8}$$

Furthermore, the r.h.s of Eq. (6) must be positive. If this is not the case, the phase transition is of first order [23].

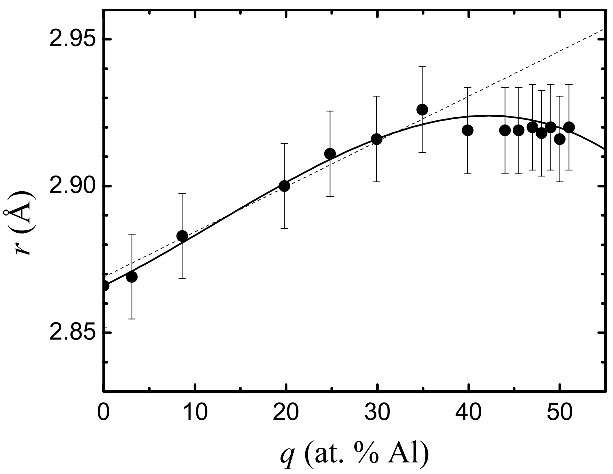

Fig. 1. The lattice parameter of disordered FeAl alloys as a function of Al concentration. The full line is the fit to Eq. (9), and the dashed straight line corresponds to the fit used in Ref. [27], dots are the experimental data Ref. [26].

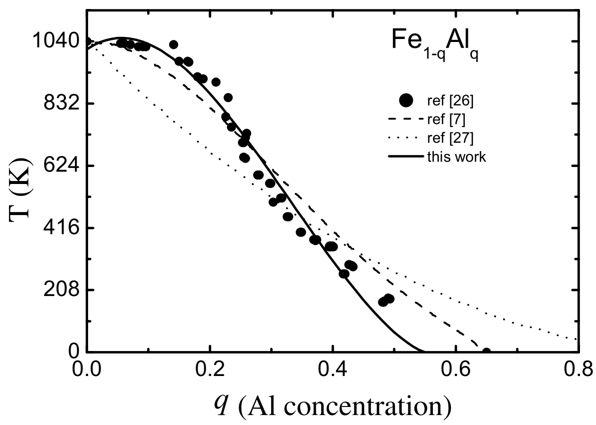

Fig. 2. Magnetic transition temperature as a function of Al concentration, the line is a fit as described in the text. Dots are the experimental data in Ref. [26], dashed line is the fitting in Ref. [7], and the dotted one is the result without superexchange interaction in Ref. [27].

3. Results

The variation of the bcc lattice parameter $r(q)$ versus the aluminum concentration q, reported by several authors [24–26] is shown in Fig. 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 Fig. 1, a deviation is observed between the experimental data and the linear model, especially for the $q > 0.25$ concentrations. Thus, the data can be best least-squares fitted with a slight cubic dependence as

$$r(q) = a_0 + a_1 q + a_2 q^2 + a_3 q^3, \tag{9}$$

where $a_0 = 2.866$ Å, $a_1 = 0.147$ Å, $a_2 = 0.247$ Å and $a_3 = -0.681$ Å.

The dilution of the iron with aluminum atoms produces a reduction in the exchange interaction. In a first approximation Pérez Alcázar et al. [27] considered that the lattice constant r dependence of the exchange interaction J is linear. Therefore, we suggest that the relationship between J_1 and q has the form

$$J_1(q) = J_0(1 + A\,q + B\,q^2 + C\,q^3), \tag{10}$$

where A, B, and C are theoretical parameters to be fitted to experimental data [27]. Using $J_0 = 12.7$ meV and applying a careful adjustment to the experimental data, one gets $A = 1.65$, $B = -4.90$ and $C = -0.35$. The quadratic and cubic terms correct the theoretical prediction without the need for introduction of the superexchange interaction [7]. We can justify the functional dependence of the exchange integral J_1 on distance r by assuming the same behavior of exchange interaction as in iron-nickel alloys [28,29].

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 have been previously reported in the literature. The recursion relation (8) 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 with the site-diluted Ising model are presented in Fig. 2 for a

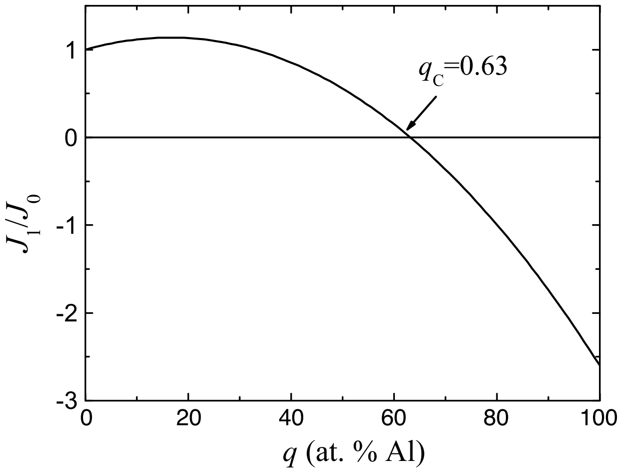

Fig. 3. Normalized exchange interaction as a function of the Al concentration.

bcc lattice and, in particular, we compare our results with the experimental data [7,14,25,26]. In contrast to other works in the literature [14,27,30] (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 $q > 0.3$ [14,30]. On the other hand, the simple cubic dependence on q for J_1 and the obtained results suggest that there is no need of a dependence with a super-exchange interaction, as proposed by the authors Dias and Plascak [14], or to describe 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 ($T_C = 1040$ K) [7]. On the other hand, when is increased the concentration of Al atoms from $q = 0.2$ to $q = 0.54$ 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 decreasing in transition temperature as a function of q. On the other hand, the FeAl alloy tends to have transition temperatures close to that of pure Fe ($T_C = 1040$ K) for small q values ($q < 0.2$). However, as q grows, the transition temperature decreases, until for $q < 0.54$ there will only be magnetic ordering at $T = 0$. The value achieved for the reduced critical temperature was the same as that obtained by Dias et al. [7]: $k_B T_C/J_1 = 7.0606$.

We can highlight a few features of the graph of $J_1(q)$ shown in Fig. 3, the object of our proposition to the Eq. (10). It is noticed that in the range $0 < q \leq 0.165$, $J_1(q)$ increases until a maximum of $J_1(q* = 0.165) = 14.443$ meV. For $q > q*$, $J_1(q)$ 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 $T > 0$. Here, the $J_1(q)$ is similar to the superexchange interaction introduced by the authors of Ref. [7]. This ensures the fact that there is 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 say 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.

In summary, with the advantage of simplicity, the model presented here can solve the problem of describing the anomalous behavior of FeAl alloys in the region of low concentration of Al. The differential operator technique is of fundamental importance in simplifying the solution process, mainly due to the reduced computational time required to search for approximate solutions. 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.

Acknowledgments

A. S. Freitas and N. O. Moreno is grateful for the partial support provided by CAPES and CNPq. We thank A. K. Nigam for critical reading of the manuscript.

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