J Supercond Nov Magn (2013) 26:2545–2548
DOI 10.1007/s10948-012-1566-5

ORIGINAL PAPER

Magnetization of the Site-Diluted Spin 1/2 Ising Model with Interactions in a Body Centered Cubic Lattice

Augusto S. Freitas · Douglas F. de Albuquerque · N.O. Moreno

Received: 27 March 2012 / Accepted: 1 April 2012 / Published online: 21 April 2012

Abstract In this work, we study the magnetic properties of the bcc lattice via site-diluted Ising model, using the operator differential technique by employing effective field theory. The results obtained here were applied to the study of the magnetic properties of Fe–Al alloys. We propose that only ferromagnetic interaction among nearest-neighbors Fe–Fe and the dependence of the exchange parameter with the aluminum concentration is quadratic. The results for the spontaneous magnetization coincides very well with the experimental data. The critical temperature as a function of aluminum concentration qualitatively describes the experimental phase diagram. We obtain the exchange interaction which is very close to that obtained using the Bogoulibov inequality and renormalization group technique.

Keywords Ising model · EFT · Fe–Al alloy

1 Introduction

In the disordered phase, the Fe–Al 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 $q < 0.3$, that is not explained by other theoretical models. On the other hand, there are proposals of the existence of antiferromagnetic superexchange interaction, which are not supported by experimental studies [1, 2].

Information about the behavior of pure or disordered magnetic systems at the phase transition has been gathered by several experimental and theoretical studies [3–7]. In the Fe–Al alloy 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. The effective field theory (EFT) 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 [1–4]. The results are achieved by treating the effects of the surrounding spins of each of the cluster through a convenient differential operator expansion technique [1, 6].

In this work, we used the EFT technique in the site-diluted spin 1/2 Ising model to study the behavior of $Fe_{1-q}Al_q$ alloy, 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_1, in terms of an expansion up to second power of q. This approach differs from earlier works [1, 6] in literature and leads to a good agreement with the experimental data.

The outline of the remainder of the work is as follows: In Sect. 2, the model and formulations are introduced. In Sect. 3, results are presented and Sect. 4, the final results are highlighted.

A.S. Freitas (✉) · N.O. Moreno
Departamento de Física, Universidade Federal de Sergipe, 49100-000, São Cristovão, SE, Brazil
e-mail: asfisfsa@yahoo.com.br

D.F. de Albuquerque
Departamento de Matemática, Universidade Federal de Sergipe, 49100-000, São Cristovão, SE, Brazil

2 Model

The proposed Hamiltonian for a site-diluted Ising model, with interaction only between nearest neighbors, has the following form [6, 7]:

$$\mathcal{H} = -J_1 \sum_{NN} \epsilon_i \epsilon_j \sigma_i \sigma_j. \tag{1}$$

Here, $J_1 > 0$ is the exchange interaction between Fe–Fe pairs, $\sigma_i = \pm 1$ and $\epsilon_i = 1$ or 0, depending if site is occupied by Al or Fe atom. The probability distribution for the ϵ_i is given by

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

where p is the Fe percentage concentration and q is the Al percentage concentration. In a similar manner to that by [3, 6], we consider only the exchange interaction, J_1, varying linearly with q (similarly to the lattice parameter). Thus, we obtained the following expression for J_1:

$$J_1(q) = J_0\left(1 + Aq + Bq^2\right), \tag{3}$$

where A and B are theoretical parameters to be fitted to experimental data [1]. Using $J_0 = 12.7$ meV and applying a careful adjustment to the experimental data, one gets $A = 1.65$ and $B = -4.90$. The linear and quadratic terms correct the theoretical prediction without the need for introduction of the superexchange interaction. The thermal average of the magnetization, starting from the Hamiltonian, Eq. (1) is given by the equation:

$$m = \left\langle \frac{\sum_{\sigma_i=\pm 1} \sigma_i e^{-\beta \mathcal{H}_i}}{\sum_{\sigma_i=\pm 1} e^{-\beta \mathcal{H}_i}} \right\rangle. \tag{4}$$

In the above expression, we use one spin cluster, in a manner similar to [6]. In this reference, it was demonstrated that there was no significant difference between the use the one or two spin clusters. Thus, for computational simplicity, we prefer to use cluster with one spin. To calculate the magnetization, we employ the Effective Field Theory (EFT), with exchange iteration $J_{ij} = J_1$ $(K_{ij} = \beta J_{ij})$. Thus, one can write the above equation as follows [6]:

$$m = \left\langle \tanh\left(\sum_{1,j} K_{1j} \sigma_j \right) \right\rangle. \tag{5}$$

Expanding the terms of Eq. (5) by applying the differential operator technique, we have [1]:

$$m = \left\langle \prod_j \left[\cosh(K_{1j} D_x) + \sigma_j \sinh(K_{1j} D_x) \right] \right\rangle \tanh(x) \Big|_{x=0}. \tag{6}$$

After expanding the terms of the above equation and application of operators to the $\tanh(x)$, at $x = 0$, we obtain the magnetization. It can be written in polynomials terms as follows:

$$m = A_{1,1}(q,K)m + A_{1,3}(q,K)m^3 + A_{1,5}(q,K)m^5 + A_{1,7}(q,K)m^7. \tag{7}$$

From the above equation, using a computer program, we can study the behavior of magnetization as a function of temperature and the temperature versus concentration diagram of Al. From Eq. (7), to obtain the critical temperature, when $m \to 0$, we must solve the equation $A_{1,1}(q, K_c) = 1$. The phase diagram T versus q is obtained from the equation above, with $A_{1,1}(q, K) = 1$, where through this, one can find the critical concentration of Al atoms for which the transition temperature will be zero and the magnetic order is broken.

3 Results

With the expression for the magnetization in hand, Eq. (7), the next step is to obtain the T–q, M–q and M–T diagrams and study the magnetic behavior of the Fe–Al alloy near the anomalous region; the Al concentration $q < 0.3$. In general, the theoretical models used to describe the behavior of Fe–Al can only obtain acceptable results for $q > 0.3$ [1, 2]. To solve the problem, [6] introduces a superexchange interaction, in contrast with Eq. (3), to describe the interactions among second neighbors of Fe atoms, however, disagreement in the range $q < 0.3$ continued. We trace of magnetization diagram, see Fig. 1.

For very small q values ($q < 0.2$), the Fe–Al alloy tends to have transition temperatures close to that of pure Fe ($T_c = 1040$ K) [6], as shown in Fig. 2. As q grows, the transition temperature decreases, until for $q < 0.54$ (AL concentration less than 54 %), the percolation threshold is reached:

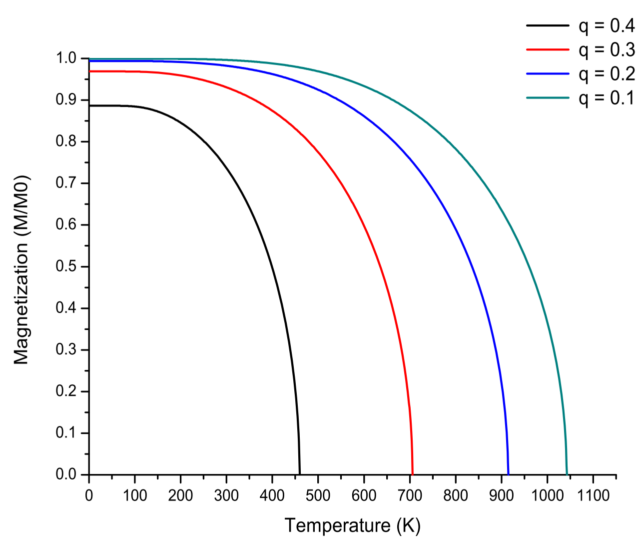

Fig. 1 Diagram of the magnetization as a function of temperature. When the Al atoms concentration increases, the reduced magnetization decreases, until the percolation threshold there is no spontaneous magnetization. For $q = 0.4$, there is a sharp drop in magnetization

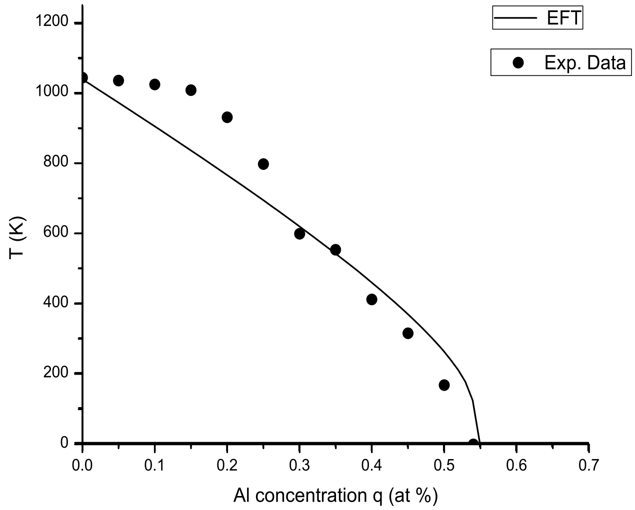

Fig. 2 Temperature as a function of Al concentration. *Dots* are the experimental data, [6], and the *line* is a fit as described in the text. We see that a better agreement between theory and experiment is obtained for $q > 0.3$

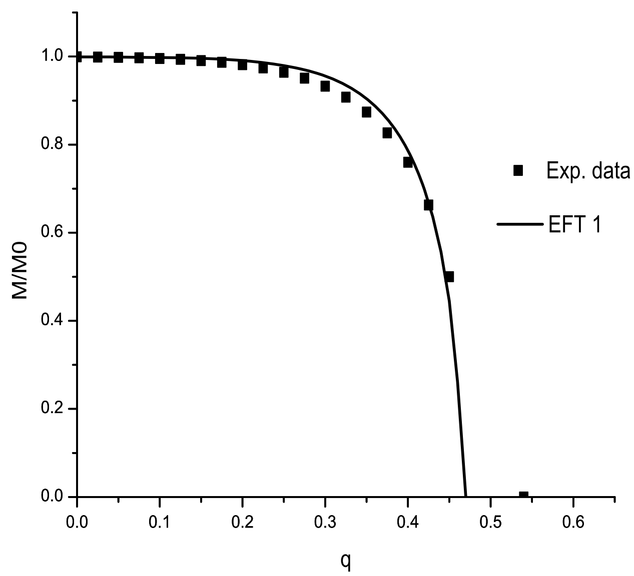

Fig. 3 Magnetization as a function of concentration, in ambient temperature. The magnetization remains constant until the vicinity of the critical concentration, when it decreases to cancel, characterizing a phase transition. The experimental data were obtained in [2]

There will only be magnetic ordering at $T = 0$. The next step was to check how it behaves the transition temperature as q varies, trying to compare the theoretical results with experimental data. From the equation for magnetization, we plot the graph of the temperature as a function of concentration and a graph of magnetization versus concentration in ambient temperature (in Figs. 2 and 3).

The diagrams shown in Figs. 1 and 2 were created based on the exchange interaction introduced by Eq. (3), based on the expression for magnetization in Eq. (7). The behavior of the reduced magnetization, shown in Fig. 1, is similar to that found in [3, 4], since the dependence of M/M_0 with T does not depend on a specific value of the q concentration. The scenario changes when we consider the dependence of critical temperature with q. The expression of $T_c(q)$ is crucial to determine a good agreement between theory and experimental data.

The large discrepancy between the experimental data and theoretical model we propose takes only in the $0.05 < q < 0.25$ interval. In other studies [1, 5], with the dependence linear of $T_c(q)$, this range is $q = 0$ to $q = 0.3$. This indicates that not only the first power of q should be taken in the account of the $T_c(q)$. This is most evident when we study the behavior of the reduced magnetization as function of the Al concentration. The T value is relatively low, considering the T–q diagram in Fig. 2. The greatest disagreement, when we observe Fig. 3, is when q is approaches its critical value, the percolation threshold, when the reduced magnetization goes to zero. We believe that it is not necessary to assume a superexchange interaction, since that the dependence of J with q is modified, i.e., do not hold varying linearly with q. This becomes clear when you see how the magnetization varies with q and T in Figs. 1 and 3. It remains constant until there is a large decrease when approaching the critical threshold, behavior that is very different from linearity. If this variation were linear, there would be a decrease in equal amounts as it reaches the critical temperature or concentration of Al atoms. That is not the case even T–q diagram, Fig. 2, although the theoretical prediction is a linear behavior when $q < 0.3$, the experimental data show, in Fig. 2 that behavior is closer to something quadratic or cubic.

The value achieved for the reduced critical temperature was the same as that obtained by [6]: $K_b T_c/J = 7.0606$. Attempts to solve the problem of anomalous behavior in the region $q < 0.3$ proposes an antiferromagnetic superexchange interaction in this range. However, such reports to [7]; there is no evidence for trial of ensuring this theoretical treatment [8, 9]. Treatments involving other theoretical models have attempted to resolve the issue, but did not succeed so far.

4 Conclusions

Our study shows that the use of an exchange interaction which depends on powers of concentration of Al, quadratic rather than linear, fits well to the experimental results, without the need to introduce a superexchange interaction. All graphs show a good agreement between experiment and theory, especially for the value of the critical concentration of Al atoms.

Acknowledgements We thank the financial support provided by CAPES.

References

1. Pérez Alcàzar, G.A., Plascak, J.A., Galvão da Silva, E.: Phys. Rev. B **34**, 1940 (1986)
2. Salazar, M., Zamora, L.E., Pérez Alcazar, G.A., Plascak, J.A.: Physica B **320**, 236 (2002)
3. Restrepo, J., Gonzalez, J.M., Pérez Alcazar, G.A., Plascak, J.A.: J. Appl. Phys. **81**(8), 5270 (1997)
4. Santos-Filho, J.B., Moreno, N.O., de Albuquerque, D.F., de Arruda, A.S.: Physica B **398**, 294 (2007)
5. Plascak, J.A., Zamora, L.E., Pérez Alcazar, G.A.: Phys. Rev. B **61**(5), 236 (2000)
6. Dias, D.A., Ricardo de Sousa, J., Pascak, J.A.: Phys. Lett. A **373**, 3513 (2009)
7. Sato, H., Arrot, A.: Phys. Rev. **114**, 1427 (1959)
8. Shukla, P., Wortis, M.: Phys. Rev. B **21**, 159 (1980)
9. Grest, G.S.: Phys. Rev. B **21**, 165 (1980)