Journal of Magnetism and Magnetic Materials 361 (2014) 137–139

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

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

Fe–Mn alloys: A mixed-bond spin-1/2 Ising model version

A.S. Freitas [a], Douglas F. de Albuquerque [a,b,*], N.O. Moreno [a]

[a] Departamento de Física, Universidade Federal de Sergipe, 49100-000 São Cristovão, SE, Brazil
[b] Departamento de Matemática, Universidade Federal de Sergipe, 49100-000 São Cristovão, SE, Brazil

ARTICLE INFO

Article history:
Received 2 August 2013
Received in revised form
3 January 2014
Available online 2 March 2014

Keywords:
Fe–Mn alloy
Ising model
EFT

ABSTRACT

In this work, we apply the mixed-bond spin-1/2 Ising model to study the magnetic properties of Fe–Mn alloys in the α phase by employing the effective field theory (EFT). Here, we suggest a new approach to the ferromagnetic coupling between nearest neighbours Fe–Fe that depends on the ratio between the Mn–Mn coupling and the Fe–Mn coupling and of second power of the Mn concentration q in contrast to linear dependence considered in the other articles. Also, we propose a new probability distribution for binary alloys with mixed-bonds based on the distribution for ternary alloys and we obtain a very good agreement for all considered values of q in T–q plane, in particular for $q > 0.11$.

1. Introduction

The effect of diluting a magnetic system by replacing some of the magnetic atoms with nonmagnetic atoms has attracted the attention of many researchers and over recent years the theoretical and experimental studies of randomly diluted magnetic systems have contributed to a significant and expressive group of works (see Refs. [1–7] and references therein for more details). In particular, these studies are motivated by a series of theoretical problems associated with disordered magnetic systems. In this context, several analytical and computational approaches have been developed in order to treat such systems [8–10] and various approximations within the real-space renormalization group method have been developed to study the critical behaviour of pure and random diluted spin systems [11–15]. Mean-field renormalization group (MFRG) method [12] is the simplest scheme for constructing a regular renormalization group mapping by using closed-form classical equations for the order parameter of the system. However, MFRG has been applied to a variety of systems with discrete and continuous degrees of freedom for the study of cooperative phenomena and phase transitions [11,16].

In this work, we consider the Effective-Field Theory (EFT) developed by Honmura and Kaneyoshi [17], which has been applied to a great variety of disordered magnetic systems [18]. Based on the identities of Callen and Suzuki [19,20] the EFT technique has been applied to the study of critical phenomena in classical and quantum spin models which display first and second-order phase transitions as well tricritical points in the phase diagram and has provided useful qualitative and quantitative insights into the critical behaviour of these systems with relative success [15,18,21–23]. These results have been obtained by treating the effects of the surrounding spins of each cluster through a convenient differential operator expansion technique introduced in the literature by Honmura and Kaneyoshi [17,24] taking all relevant self-spin correlations into account and including the contribution of the set of spins. EFT provides a hierarchy of approximations to obtain thermodynamic properties of magnetic models. One can continue these series of approximations and consider larger and larger clusters and as a consequence better results are obtained. The exact solution would be obtained by considering an infinite cluster. However, by using relatively small clusters that contain the topology of the lattice, one can obtain a reasonable description of thermodynamic properties [15,22].

The Fe–Mn alloys in the α phase (α-Fe–Mn) have a bcc lattice structure [7,25–28] which is observed up to about 20 at% Mn. When the Mn concentration q increases, the magnetization linearly decreases up to $q < 0.11$. The average hyperfine field decreases linearly with Mn concentration q up to 20 at% Mn [25,26]. The magnetic properties of the Fe–Mn alloys have been studied extensively by means of Mössbauer effect, nuclear magnetic resonance, magnetization and other experimental techniques [25,26,29]. Interesting properties of this alloys emerge from other structural phases such as γ-Fe–Mn (fcc structure) and, in this phase, the Fe–Mn alloys presents antiferromagnetic and glassy behaviour [28,29]. Theoretic and experimental studies shows that the magnetic ground state strongly depends on the lattice

* Corresponding author.
E-mail address: douglas@ufs.br (D.F. de Albuquerque).

http://dx.doi.org/10.1016/j.jmmm.2014.02.084
0304-8853

parameter and this is a function of the Mn concentration (See ref. [28, and references therein]).

In Peña Lara et al. [30] the probability distribution for exchange interaction J_{ij} depends on the bonds J_1 ferromagnetic Fe–Fe atoms, $-\gamma J_1$ and $-\lambda J_1$ bonds antiferromagnetic for Mn–Mn and Fe–Mn, respectively. On the other hand, $\gamma = |J_{MnMn}|/|J_{FeFe}|$ and $\lambda = |J_{FeMn}|/|J_{FeFe}|$ have been used in the literature by Paduani et al. [25] with γ=0.05 and λ=0.03 [3,30]. More recently, different probability distributions for Fe–Mn–Al and Fe–Ni–Mn alloys have been considered [3,30–32] due to the asymmetric nature of these alloys. Since the probability distribution for the exchange interactions in the Fe–Mn is asymmetric we assume that the distribution is analogous to the ternary alloys with some subtle differences (for example, the *2pq* term for binary alloys where p and q are both the Fe and Mn concentration, respectively. See Ref. [3,30] for more details) and we use it for the present work. Here, we consider the technique generally used to describe disordered magnetic materials, namely, the diluting picture, and we studied the phase diagram in the T–q plane for Fe–Mn alloys. On the other hand, we also propose a new probability distribution for binary alloys based on the distribution for ternary alloys.

The outline of the remainder of this paper is as follows: the model and formalism are described briefly in Section 2, the results and discussion are presented in Section 3 and conclusions are presented in Section 4.

2. Model and formalism

We consider a mixed-bond spin-1/2 Ising model on a bcc lattice. The Hamiltonian of the system is given by

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij} S_i^z S_j^z, \tag{1}$$

where the summation is performed over all pairs of the nearest-neighbors sites $\langle i,j\rangle$ and the quantities S_i^z are isotropically interacting classical spins localized on the sites i ($S_i^z = \pm 1$).

By employing the EFT with differential operator technique on a cluster comprising just a single selected spin labelled S_1^z and the neighboring spins with which it directly interacts. The average magnetization per spin is given by

$$\langle S_1^z\rangle = \left\langle \prod_j e^{K_{1j} S_j^z D_x} \right\rangle f(x)|_{x=0},$$

where $D_x \equiv \partial/\partial x$, $K_{1j} \equiv \beta J_{1j}$, $\beta \equiv 1/k_B T$ and $f(x) = \tanh(x)$.

By employing the van der Waerden identity for spin $S = 1/2$ [33], one gets

$$\langle S_1^z\rangle = \left\langle \prod_j^Z [\cosh(K_{1j} D_x) + S_j^z \sinh(K_{1j} D_x)] \right\rangle f(x)\Big|_{x=0}, \tag{2}$$

where Z is the coordination number (Z=8 for bcc lattice). In the vicinity of the second-order phase transition, $m_z \simeq 0$. Then performing the configurational average at the Eq. (2) (here, denoted by $m_z = \langle\langle S_1^z\rangle\rangle_c$) and by expanding up to first order in this parameter, we obtain

$$m_z = A_1(q, K_1) m_z + \mathcal{O}(m_z^3),$$

with $K_1 \equiv \beta J_1$. $A_1(q, K_1)$ can be calculated by applying the relation [34]

$$2\sinh(a D_x) f(x) = f(x+a) - f(x-a),$$

where A_1 is a very long function of q and K after performing configuration averaging and we do not believe it to be necessary to put here.

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 [24,34]. Since the magnetization m_z goes to zero continuously, a second-order transition line is given by the following equation:

$$A_1(q, K_1) = 1. \tag{3}$$

In next section, we present some important results and remarks for the present work.

3. Remarks and discussion

In order to study the T–q phase diagram of disordered Fe–Mn alloys on a bcc lattice, we follow the same procedure of the Ref. [35]. Whereas the introduction of Mn atoms on alloy produces a variation in the exchange interaction, then we suggest ferromagnetic J_1 that obeys the following probability distribution:

$$P(J_1) = (1-q)\delta(J_1 - J_+) + q\,\delta(J_1 - J_-), \tag{4}$$

with

$$J_\pm(q) = J_0 \cdot \left(1 \pm \frac{\gamma}{\lambda}(q+q^2)\right), \tag{5}$$

where $J_0 = 12.8$ meV is the ferromagnetic coupling for pure iron (see [25,36]) and $\gamma/\lambda = |J_{MnMn}|/|J_{FeMn}| \approx 1.67$. This result indicates that the Mn–Mn antiferromagnetic coupling is greater than the Fe–Mn coupling and has a significant influence with the experimental results according to the spin-1/2 Ising model. Therefore, we suggest that the functional dependence of the coupling $J_\pm$ on Mn concentration q has the same behavior of exchange interaction as in iron–nickel alloys [37–39]. On the other hand, the lattice parameter, $r(q)$, for the Fe–Mn alloys remains approximately constant for $q \leq 0.11$ and increases linearly up to $q = 0.2$. This change of $r(q)$ implies a variation in the exchange interaction J_1 suggesting a reduction as function of q as the atom concentration of Mn increases above q=0.11. In other words, $J_\pm$ grows to low values of q concentrations of Mn atoms and decreases for $0.11 < q < 0.2$.

At this point, we consider a numerical treatment which can be done without great effort to obtain the phase diagram by using Eq. (3), J_1 defined by Eq. (5) and the experimental data [25,26,29,40]. Fig. 1 shows the phase diagram T–q for $0 \leq q \leq 0.2$ obtained by the recurrence relationship (3). We observe that there is excellent agreement between the experimental data and our theoretical fit for the range considered. Such result shows that our assumptions are consistent. Parameters γ and λ are important in the present

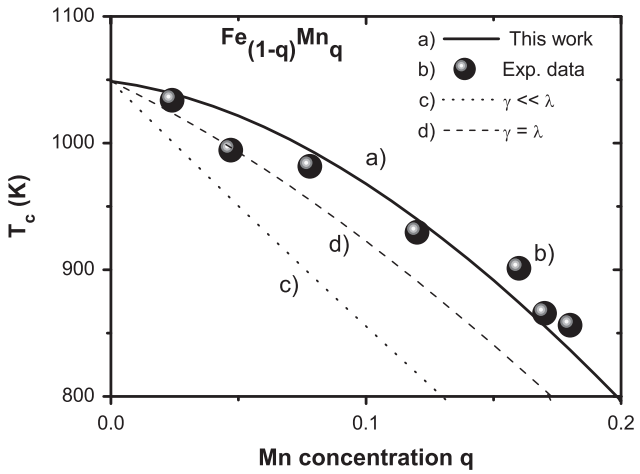

Fig. 1. Phase diagram in the T–q plane. a) is a fit as described in the present work. d) represents the Eq. (3) with $\gamma = \lambda$ and c) line $\gamma \ll \lambda$ (γ/λ=0.01) for spin-1/2 Ising model, respectively. b) solid circles are the experimental data, Refs. [25,26,29,40].

work and are highlighted in Fig. 1 at the same time as we realize that when $\gamma \ll \lambda$ and $\gamma = \lambda$ the critical temperature decreases linearly and quasi-linearly, respectively. On the other hand, for spin-1/2 Ising model there is a smooth decrease dT_c/dq when $\gamma/\lambda \approx 1.67$. This result is in agreement with the phenomenological predictions cited in Refs. [6,36,41], in particular for $q < 0.2$ indicating that strong ferromagnetic coupling J_1 influences the spontaneous magnetization of the Fe–Mn alloys.

4. Conclusions

The purpose of this study was to investigate the phase diagram in the T–q plane of the diluted spin-1/2 Ising model on a bcc lattice within the framework of the EFT based on a probability distribution technique that accounts for the self-spin correlations. We observe that our results are qualitatively and quantitatively consistent with the experimental data for all considered concentration range of Mn atoms even when employing the simplest version on a cluster comprising just a single selected spin, in contrast to other approaches contained in the literature carried out using only the linear dependence of the exchange constant as a function of Mn atoms [25,26,29]. Therefore, the applicability of the one-spin cluster EFT scheme for mixed-bond spin-1/2 Ising model adequately describes the behaviour of the phase diagram in the T–q plane for Fe–Mn in the α phase with simple approach and good agreement between theory and experimental data.

In synthesis, our result leads to a more transparent physical picture of the problem as compared with others presented in the literature based on the mean field theory.

Acknowledgments

A. S. Freitas and N. O. Moreno are grateful for the partial support provided by CAPES and CNPq, respectively.

References

[1] R. Stinchcombe, Phase Transitions and Critical Phenomena, vol. 7, Academic Press, New York, 1983.
[2] P.H.R. Barbosa, E.P. Raposo, M.D. Coutinho-Filho, Phys. Rev. Lett. 91 (2003) 197207, http://dx.doi.org/10.1103/PhysRevLett.91.197207.
[3] D.P. na Lara, J.E. Diosa, C.A. Lozano, Phys. Rev. E 87 (2013) 032108, http://dx.doi.org/10.1103/PhysRevE.87.032108.
[4] K.A.P. de Lima, J.B. Brito, P.H.R. Barbosa, E.P. Raposo, M.D. Coutinho-Filho, Phys. Rev. B 85 (2012) 064416, http://dx.doi.org/10.1103/PhysRevB.85.064416.
[5] D.A. Dias, J.A. Plascak, Phys. Lett. A 375 (2011) 2089–2093, http://dx.doi.org/10.1016/j.physleta.2011.04.022.
[6] O. Beutler, R. Kirsch, M.J. Prandolini, W.D. Brewer, J. Kapoor, P.J. Jensen, S. Frota-Pessa, D. Riegel, Europhys. Lett. 70 (2005) 520, http://dx.doi.org/10.1209/epl/i2005-10013-7.
[7] M. Mizrahi, A.F. Cabrera, S.M. Cotes, S.J. Stewart, R.C. Mercader, J. Desimoni, Hyperfine Interact. 156–157 (2004) 541, http://dx.doi.org/10.1023/B:HYPE.00000-43275.05430.16.
[8] W. Wolf, Braz. J. Phys. 30 (4) (2000) 794–810, http://dx.doi.org/10.1590/S0103-97332000000400030.
[9] G.A.P. Alcazar, J.A. Plascak, E.G. Da Silva, Phys. Rev. B 34 (3) (1986) 1940, http://dx.doi.org/10.1103/PhysRevB.34.1940.
[10] R.A. Dos Anjos, J.R. Viana, J.R. De Sousa, J.A. Plascak, Phys. Rev. E 76 (2). http://dx.doi.org/10.1103/PhysRevE.76.022103.
[11] D.F. de Albuquerque, I.P. Fittipaldi, J.R. de Sousa, Phys. Rev. B 56 (1997) 13650, http://dx.doi.org/10.1103/PhysRevB.56.13650.
[12] J.O. Indekeu, A. Maritan, A.L. Stella, Phys. Rev. B 35 (1) (1987) 305, http://dx.doi.org/10.1103/PhysRevB.35.305.
[13] N. Benayad, A. Benyoussef, N. Boccara, E. Kenz, J. Phys. C 21 (1988) 5747, http://dx.doi.org/10.1088/0022-3719/21/34/011.
[14] T.W. Burkhardt, J.M.J. van Leeuven, Progress and Problems in Real Space Renormalization Group, Springer, Berlin, Heidelberg (1982) http://dx.doi.org/10.1007/978-3-642-81825-7_1.
[15] D.F. de Albuquerque, E. Santos-Silva, N.O. Moreno, J. Magn. Magn. Mater. 321 (2009) L63–L64, http://dx.doi.org/10.1016/j.jmmm.2009.05.001.
[16] A.S. Freitas, D.F. de Albuquerque, I.P. Fittipaldi, N.O. Moreno, J. Appl. Phys. 113 (2013) 093903, http://dx.doi.org/10.1063/1.4794090.
[17] R. Honmura, T. Kaneyoshi, J. Phys. C 12 (19) (1979) 3979–3992, http://dx.doi.org/10.1088/0022-3719/12/19/016.
[18] I.P. Fittipaldi, D.F. de Albuquerque, J. Magn. Magn. Mater. 107 (1992) 256, http://dx.doi.org/10.1016/0304-8853(92)90779-N.
[19] H.B. Callen, Phys. Lett. (1963), http://dx.doi.org/10.1016/0031-9163(63)90344-5 (p. 161).
[20] H. Suzuki, Phys. Lett. (1965), http://dx.doi.org/10.1016/0031-9163(65)90978-9 (p. 267).
[21] I.P. Fittipaldi, E.F. Sarmento, T. Kaneyoshi, Physica A 186 (3–4) (1992) 591–607, http://dx.doi.org/10.1016/0378-4371(92)90219-G.
[22] J.R. de Sousa, D.F. de Albuquerque, A.S. de Arruda, Physica A 391 (2012) 3361, http://dx.doi.org/10.1016/j.physa.2012.01.049.
[23] E. Costabile, J.R. Viana, J.R. de Sousa, J.A. Plascak, Physica A 393 (2014) 297, http://dx.doi.org/10.1016/j.physa.2013.09.003.
[24] T. Kaneyoshi, I.P. Fittipaldi, R. Honmura, T. Manabe, Phys. Rev. B 24 (1) (1981) 481, http://dx.doi.org/10.1103/PhysRevB.24.481.
[25] C. Paduani, J.A. Plascak, E. Galvão da Silva, Phys. Rev. B 44 (17) (1991) 9715, http://dx.doi.org/10.1103/PhysRevB.44.9715.
[26] C. Paduani, E. Galv ao da Silva, G.A. Perez Alcázar, J. Appl. Phys. 70 (1991) 7524–7531, http://dx.doi.org/10.1063/1.349704.
[27] N.I. Kulikov, C. Demangeat, Phys. Rev. B 55 (1997) 3533, http://dx.doi.org/10.1103/PhysRevB.55.3533.
[28] M. Ekholm, I.A. Abrikosov, Phys. Rev. B 84 (2011) 104423-1–104423-16, http://dx.doi.org/10.1103/PhysRevB.84.104423.
[29] G. Aeppli, S.M. Shapiro, R.J. Birgeneau, H.S. Chen, Phys. Rev. B 28 (1983) 5160, http://dx.doi.org/10.1103/PhysRevB.28.5160.
[30] D. Pe na Lara, G.A. Pérez Alcázar, L.E. Zamora, J.A. Plascak, Phys. Rev. B 80 (2009) 014427, http://dx.doi.org/10.1103/PhysRevB.80.014427.
[31] J. Restrepo, G.A. Pérez Alcázar, Phys. Rev. B 61 (9) (2000) 5880–5883, http://dx.doi.org/10.1103/PhysRevB.61.5880.
[32] L.E. Zamora, G.A. Pŕez-Alcázar, A. Bohórquez, J.F. Marco, J.M. González, J. Appl. Phys. 82 (12) (1997) 6165–6169, http://dx.doi.org/10.1063/1.366500.
[33] J.W. Tucker, J. Phys. A: Math. Gen. 27 (1994) 659, http://dx.doi.org/10.1088/0305-4470/27/3/011.
[34] D.F. de Albuquerque, S.L. Alves, A.S. de Arruda, Phys. Lett. A 346 (2005) 128, http://dx.doi.org/10.1016/j.physleta.2005.07.060.
[35] A.S. Freitas, D.F. de Albuquerque, N.O. Moreno, Physica A 391 (2012) 6332, http://dx.doi.org/10.1016/j.physa.2012.06.068.
[36] J.A. Plascak, L.E. Zamora, G.A. Pérez Alcazar, Phys. Rev. B 61 (5) (2000) 3188–3191, http://dx.doi.org/10.1103/PhysRevB.61.3188.
[37] M. Hatherly, K. Hirakawas, R. Lowde, J. Mallettg, M. Stringfellow, B. Torrie, Proc. Phys. Soc. 64 (1964) 55, http://dx.doi.org/10.1088/0370-1328/84/1/309.
[38] U. Krey, Z. Phys. B 31 (1978) 247, http://dx.doi.org/10.1007/BF01352349.
[39] S.N. Kaul, Phys. Rev. B 27 (11) (1983) 6923–6933, http://dx.doi.org/10.1103/PhysRevB.27.6923.
[40] N. Cabañas, N. Akdut, J. Penning, B.C.D. Cooman, Metall. Mater. Trans. A 37A (2006) 3305–3315, http://dx.doi.org/10.1007/BF02586165.
[41] D.A. Dias, J.R. de Sousa, J.A. Plascak, Phys. Lett. A 373 (39) (2009) 3513–3515, http://dx.doi.org/10.1016/j.physleta.2009.07.086.