Diluted and random-bond Ising model: Application to the Fe-Mn-Al alloys

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A quenched disordered Ising model with a distribution function that includes dilution and random bonds is studied through the mean-field renormalization-group approach. The phase diagram is obtained, and the results are applied to Fe-Mn-Al alloys. Fittings of the experimental phase diagram and the reduced mean hyperfine field at room temperature are shown to be better than those previously obtained through a single-site diluted model.

The magnetic properties of Fe-Mn-Al alloys in the disordered phase have been recently investigated through the Mössbauer technique.[1,2] The magnetic phase diagram at room temperature has been obtained as a function of Al concentration q and Mn concentration x. For $q<0.5$ and $x<0.45$ the alloys have bcc structure and undergo a ferromagnetic-paramagnetic transition with the mean hyperfine field $\bar{H}$ going continuously to zero at the critical concentration. A site-diluted Ising model has also been proposed for these alloys and could account for the main magnetic properties of the Fe-Mn-Al system. In particular, quite good fits of the experimental phase diagram and mean hyperfine field for $x<0.2$ and $q>0.3$ have been obtained by taking the same theoretical parameters used to fit the results of the binary Fe-Al alloy.[3] However, for low Al concentrations, which implies a higher Mn concentration to destroy the order at room temperature, the experimental results go to zero more rapidly than the theoretical ones (for details see Refs. 1 and 2). This discrepancy can be associated with the fact that as x increases, Mn can effectively exhibit an extra-competitive antiferromagnetic interaction with Fe atoms, as has been reported for the binary Fe-Mn alloy.[4,5] Such interaction is not present in the theoretical model of Ref. 1 once it only considers dilution.

In this Brief Report we propose a quenched disordered Ising model with a new distribution function that includes dilution and random bonds in order to take into account the antiferromagnetic interactions that should be induced by the Mn atoms.

Let us first consider a system described by a nearest-neighbor spin Hamiltonian given by

$$H=-\sum_{\langle i,j\rangle}K_{ij}\sigma_i\sigma_j\,, \tag{1}$$

where $K_{ij}=\beta J_{ij}$ is the reduced coupling constant of the disordered exchange interaction between the pair of nearest-neighbor spins $\langle i,j\rangle$ and $\sigma_i=\pm 1$. We assume the following probability distribution for each bond:

$$P(K_{ij})=p\delta(K_{ij}-K)+q\delta(K_{ij})+x\delta(K_{ij}+\alpha K)\,, \tag{2}$$

with $p+q+x=1$.

In order to study the phase diagram of the above model we employ the mean-field renormalization-group (MFRG) (Ref. 6) procedure by considering the simplest choice for the clusters, namely, one- and two-spin clusters. In some limiting cases this model has been previously treated by the MFRG. Droz, Maritan, and Stella[7] have studied the bond-diluted Ising model ($x=0$) and the symmetric random-bond Ising model ($q=0$ and $\alpha=1$) while the asymmetric random bond ($\alpha\neq 1$) has been treated by Lyra and Coutinho.[8] In this case, second-order lines separate paramagnetic, ferromagnetic, antiferromagnetic, and spin-glass phases. The phase diagram is symmetric for $\alpha=1$ and presents reentrancies in the ferromagnetic or antiferromagnetic boundaries depending on the value of α. In all models it has been shown that this choice of smaller clusters is strictly equivalent to the Bethe-Peierls approximation.

The Hamiltonian for the one- and two-spin clusters are given, respectively, by

$$H_1=-\sum_{i=1}^{z}K_i'b_i'\sigma_1\,, \tag{3}$$

$$H_2=-K\sigma_1\sigma_2-\sum_{i=1}^{z-1}K_{1i}b_{1i}\sigma_1-\sum_{j=1}^{z-1}K_{2j}b_{2j}\sigma_2\,, \tag{4}$$

where z is the coordination number of the lattice and b_i' and b_{mj} ($m=1,2$) are the effective fields acting on the boundary of the respective cluster. The magnetization for each block can be evaluated straightforwardly and for small effective fields we get

$$\langle\sigma_1\rangle=\sum_{i=1}^{z}K_i'b_i'\,, \tag{5}$$

$$\langle\sigma_2\rangle=\sum_{i=1}^{z-1}K_{1i}b_{1i}+\tanh K_{12}\sum_{j=1}^{z-1}K_{2j}b_{2j}\,, \tag{6}$$

where $\langle\sigma_1\rangle$ and $\langle\sigma_2\rangle$ are the magnetizations per spin of the one- and two-spin clusters, respectively.

To perform the configurational average $\overline{\langle\cdots\rangle}$ we assume that K_i and b_i are independent random variables

with the following symmetry conditions for the effective fields associated with the magnetization and the staggered magnetization: $\overline{b_i'}=b'$, $\overline{b_{1j}}=b$, $\overline{b_{2j}}=\pm b$, where here, and in what follows, the upper (lower) sign holds for the ferromagnetic (antiferromagnetic) order parameters. We then get

$$\langle\sigma_1\rangle=z(p'-\alpha'x')K'b', \tag{7}$$

$$\langle\sigma_2\rangle=[p(1\pm\tanh K)+q + x(1\mp\tanh\alpha K)](z-1)(p-\alpha x)Kb. \tag{8}$$

For the spin-glass order parameter the symmetry conditions are $\overline{b_i'}=0$, $\overline{b_i'b_j'}=h'\delta_{ij}$, $\overline{b_{mj}}=0$, $\overline{b_{mi}b_{lj}}=h\delta_{ml}\delta_{ij}$. These relations have been proposed by Lyra and Coutinho.[8] They differ from those of Ref. 7 by not including correlations between the random symmetry-breaking fields of the spin-glass boundary conditions. In this case, previous results for the Ising spin-glass model on the Bethe lattice are recovered. The Edwards-Anderson spin-glass order parameter for each cluster can be obtained by squaring Eqs. (5) and (6), respectively, and performing the configurational average following the appropriated symmetry-breaking conditions given above; that is

$$\overline{\langle\sigma_1\rangle^2}=z(p'+\alpha'^2x')K'^2h', \tag{9}$$

$$\overline{\langle\sigma_2\rangle^2}=[p(1+\tanh^2K)+q + x(1+\tanh^2\alpha K)](z-1)(p+\alpha^2x)K^2h. \tag{10}$$

According to the standard MFRG approach the recursion relations among the parameters of the Hamiltonian are obtained through the order parameters $\overline{\langle\sigma\rangle}$ and $\overline{\langle\sigma\rangle^2}$. It is clear that with just two equations we cannot determine the complete renormalization flow diagram in the space of the parameters of the Hamiltonian. Instead, we can study the fixed-point solutions $K'=K=K_c$ in the subspace $\alpha=\alpha'$, $p=p'$, $q=q'$, and $x=x'$ (see also Refs. 7 and 8). We then get

$$z=(z-1)[p(1\pm\tanh K_c)+q+x(1\mp\tanh\alpha K_c)], \tag{11}$$

which gives the ferromagnetic (upper sign) and antiferromagnetic (lower sign) phase boundaries and

$$z=(z-1)[p(1+\tanh^2K_c)+q+x(1+\tanh^2\alpha K_c)] \tag{12}$$

for the spin-glass boundary. For $q=0$, Eqs. (11) and (12) are identical to those obtained by Lyra and Coutinho[8] in the Ising limit and for $x=0$ we recover the equations for the diluted model studied by Droz *et al.*[7]

Figure 1 shows the phase diagram in the $\tilde{T}_c\times p$ plane with $\tilde{T}_c=k_BT_c/J$, for $z=6$ and $\alpha=1$ and different values of q. For $q>0$ the maximum concentration of ferromagnetic bonds is given by $p_M=1-q$ and the diagram is always symmetric with respect to $p_M/2$. The spin-glass line is independent of p and the width of this phase at $T=0$ is independent of q for $q<0.296$. For $q>0.296$ (this value is z dependent) the spin-glass phase disappears.

For asymmetric random bonds ($\alpha\neq1$) the phase diagrams are similar to those reported in Ref. 8. The effect of the dilution is to lower the critical temperature and for q greater than a value q^* (which depends on z and α) the spin-glass phase also disappears. Figure 2 shows a typical phase diagram for the theoretical parameters obtained for the Fe-Mn-Al alloy.

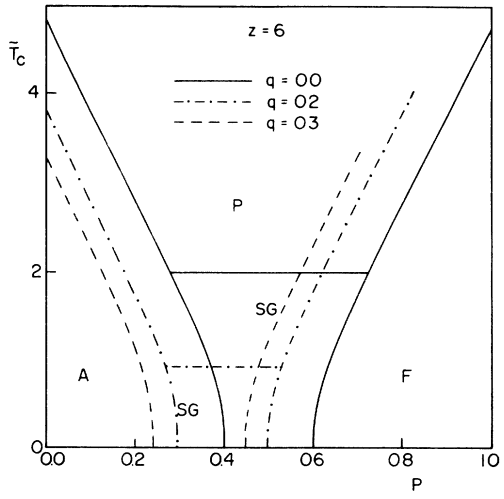

FIG. 1. Symmetric random-bond ($\alpha=1$) phase diagram for different values of q.

Next, we discuss the application of the present theoretical model to the ternary Fe-Mn-Al system. It has been shown that the Fe-Al alloys are all ferromagnetic where the Fe magnetic moment is constant and the Al atom behaves like a magnetic hole.[3,9] A site-diluted Ising model has then been proposed for this binary system and extended to the Fe-Mn-Al alloys assuming that the Mn atom behaves as the Al atom.[1] However, for Fe-Mn al-

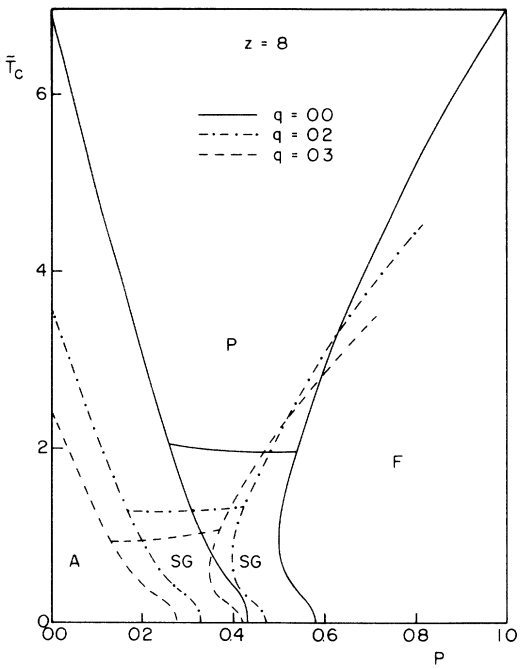

FIG. 2. Asymmetric random-bond phase diagram for different values of q and using the theoretical parameters for the Fe-Mn-Al alloys given in the text. In this case, the reentrancies appear in the ferromagnetic boundary.

loys at large Mn concentrations, it has been reported that Mn induces an antiferromagnetic interaction.[4,5] It has been argued that the discrepancy between the experimental data and the site-diluted model as the Mn concentration increases could be associated with this extra-competitive coupling.[1]

On the other hand, for $x=0$, the present approximation with the smallest clusters (one- and two-spin clusters) gives the same result for the ferromagnetic-paramagnetic phase boundary of the site- and bond-diluted Ising model (see, for example, Ref. 10). Therefore, the model given by Eqs. (1) and (2) is the easiest way to introduce this extra-competitive coupling due to Mn atoms. In this case, p, q, and x are the concentrations of Fe, Al, and Mn atoms, respectively. We assume further that $\alpha=x$ in order to enhance the antiferromagnetic interaction as the Mn concentration increases. We also consider that the exchange parameter $J=J(q)=J_1-J_0q$ changes with the Al concentration q and remains constant with the Mn concentration x (see Figs. 4 and 5 of Ref. 1).

By using the previous adjusted values for the parameters of the exchange interaction,[3] namely, $J_1=12.846$ meV and $J_0/J_1=0.95$, and assuming $\alpha=x$, we obtain curve 1 of Fig. 3. We can see that the agreement with the experimental data is now much better and indicates that the antiferromagnetic coupling seems to be relevant as the Mn concentration is increased. Figure 2 shows the full theoretical diagram with the parameters above and various values of q. We have also verified that the transition line in Fig. 3 is always from the ferromagnetic phase to the paramagnetic phase.

In order to get a further quantitative comparison of the present theoretical model with the experimental data of this ternary alloy we can use the variational method based on Bogoliubov's inequality within the pair approximation suggested by Ferreira, Salinas, and Oliveira[11] to obtain $\langle\sigma\rangle=m$. m is the ferromagnetic order parameter which is related to the mean reduced hyperfine field $\bar{H}$. The procedure is similar to that done in Refs. 3 and 10. For the present model we obtain

$$m=\tanh(\beta\gamma_s)=q\tanh(\beta\gamma_p)+p\frac{\sinh 2\beta\gamma_p}{\cosh 2\beta\gamma_p+e^{-2\beta J}}+x\frac{\sinh 2\beta\gamma_p}{\cosh 2\beta\gamma_p+e^{2\beta aJ}}, \tag{13}$$

where $(z-1)\gamma_s=z\gamma_p$. Close to the transition m, γ_s, and γ_p are very small and expanding Eq. (13) we get the same result for the ferromagnetic boundary given by Eq. (11), as expected. The curves labeled as 1 in Fig. 4 show the present fittings of the reduced mean hyperfine field as a function of q and x. Again, with the same adjusted values of J_1, and J_0/J_1, better fittings are obtained. In summary, although the present model is still a simple one, it seems that the antiferromagnetic character induced by Mn atoms are relevant in order to account for the main magnetic properties of Fe-Mn-Al alloys. Experimental work at low temperatures in order to study the possible spin-glass phase is now in progress.

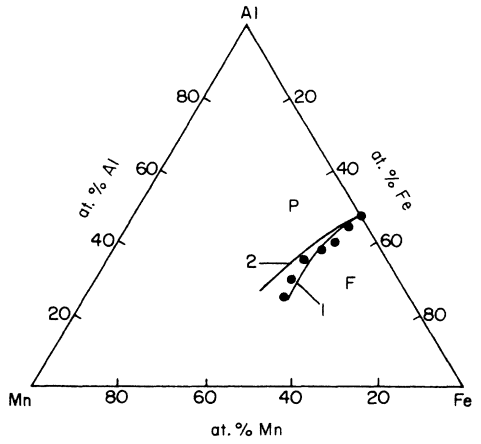

FIG. 3. Phase diagram of the ternary Fe-Mn-Al system. The dots represent the experimental results of the ferromagnetic (F) to paramagnetic (P) transition in the bcc structure. The solid lines represent the theoretical results according to the present model (line 1) and the model discussed in Ref. 1 (line 2).

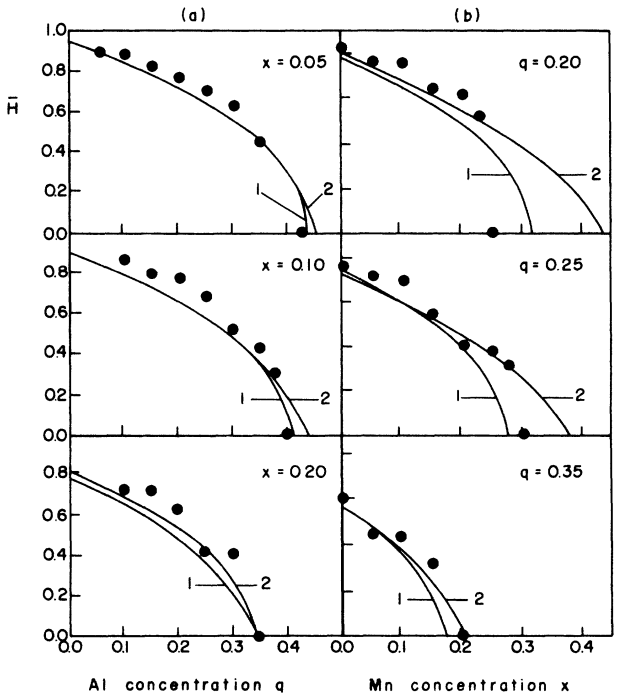

FIG. 4. Mean reduced hyperfine field $\bar{H}$ as function of (a) Al concentration q and (b) Mn concentration x. Lines 1 and 2 are the same as in Fig. 3.

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