Magnetic properties of *Pt*Fe alloys calculated by Monte Carlo methods

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A magnetic-environment model is used to calculate, by Monte Carlo methods, the critical temperatures and magnetization of dilute *Pt*Fe alloys. The diffuse unpolarized-neutron cross sections were also calculated, including the critical scattering, in both *Pt*Fe and *Pd*Fe alloy. A good agreement with experimental data was obtained for all calculations.

INTRODUCTION

A magnetic-environment model[1,2] has been recently applied, successfully, to giant-moment ferromagnets such as *Pd*Fe and *Pt*Fe dilute alloys. In those works it was shown that the interaction between magnetization clouds is properly represented by a Heisenberg model where the exchange-interaction constant decays exponentially with the separation between clouds. Using this model, several magnetic properties of *Pd*Fe alloys were calculated, such as critical temperatures, susceptibilities, neutron scattering data, and the spin-wave-stiffness constant.

The shape of magnetization clouds and the interaction constants between giant moments were calculated[2] for *Pt*Fe. In contrast with the case of *Pd*Fe, the calculated shape of the clouds of *Pt*Fe does not agree with unpolarized-neutron scattering data.[3] This indicates that some critical scattering must be present in the neutron experiment. The purpose of this paper is to use the Monte Carlo method to calculate the critical temperatures, magnetization, and neutron scattering of *Pt*Fe.

CRITICAL TEMPERATURES AND MAGNETIZATION

We have made Monte Carlo calculations in the concentration region $0.76 < c < 5$ at. % Fe where the dependence of critical temperatures of ferromagnetism with respect to concentration is linear. We considered a system of N classical spins of magnitude one obeying the following Hamiltonian:

$$H = -\frac{1}{2}\sum_{\substack{i,j \\ i\neq j}} \mathbf{S}_i\cdot\mathbf{S}_j J_{ij}(r_{ij}) - \sum_i \mathbf{B}\cdot\mathbf{S}_i \ , \tag{1}$$

where J_{ij} were calculated in Ref. 2. For a given concentration we distribute at random the N particles in a fcc lattice with periodic boundary conditions. In each Monte Carlo iteration a spin is chosen at random and its local field $\mathbf{H}$, produced by the other $N-1$ spins, is calculated.

A new direction of the spin is then chosen at random and the energy change is calculated using $\Delta E = -\mathbf{H}\cdot\Delta\mathbf{S}$. A transition to the new direction is performed with the probability $\max(1, \exp(-\Delta E/kT))$. In the cases in which no transitions are allowed we still perform a transition to a different direction which conserves the angle between $\mathbf{S}$ and $\mathbf{H}$. This transition to a state of equal energy allows the algorithm to sample a bigger volume of phase space.

For each concentration we calculated, for several temperatures, the following quantities: the energy E, the z component and the magnitude of the total magnetic moment M, the susceptibility χ (from the average fluctuation of a component of the total magnetic moment), and a quantity $\tilde{\chi}$ which coincides with χ for infinite systems and which is given by the fluctuation of the magnitude of the total moment:

$$\tilde{\chi} = \frac{\langle (M - \langle M \rangle)^2 \rangle}{NkT} \ . \tag{2}$$

The calculations were performed in the following way:

(1) To initialize the calculation at a given concentration, we create a configuration where all the spins are aligned in the same direction.

(2) In order to achieve equilibrium, we made 500 Monte Carlo steps per spin for each temperature before calculating the averages.

(3) Every two Monte Carlo steps per spin, we took the instantaneous values of the energy and of the M_z com-

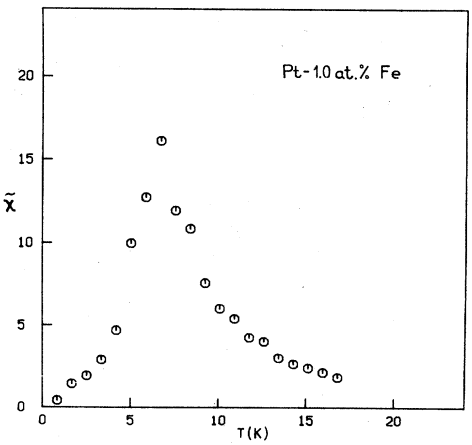

FIG. 1. Typical results of χ-vs-T values obtained by Monte Carlo calculations. Critical temperatures correspond to the maximum of χ.

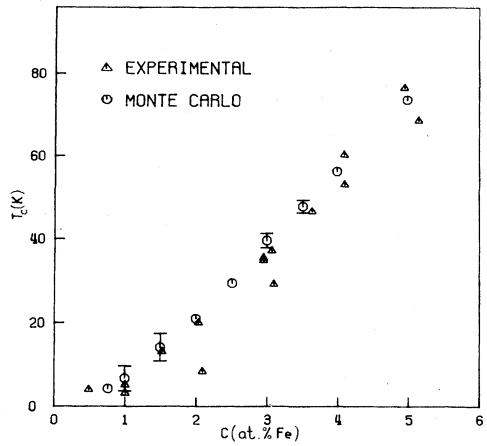

FIG. 2. Critical temperatures for the onset of ferromagnetism, as obtained with our model by Monte Carlo calculations, are compared with experimental data from Ref. 4 and other references therein.

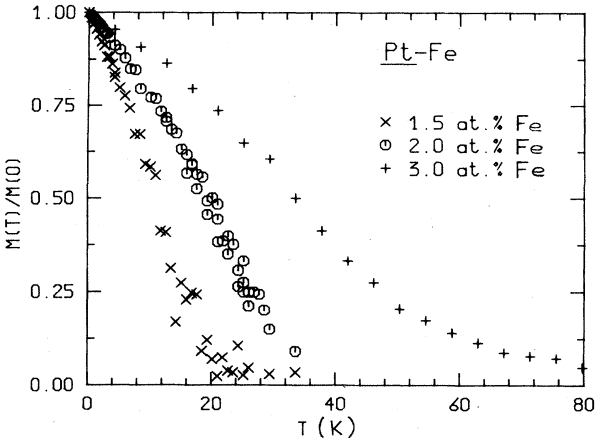

FIG. 3. Calculated magnetization values as a function of temperature, in the presence of a small applied field.

ponent of the total magnetic moment. This process was repeated 2000 times in order to calculate the averages.

(4) To make the calculations at a new temperature we took the final configuration of the preceding temperature as the initial configuration.

Two sets of calculations were performed, one with $N=100$ and $B=0$ which allowed the determination of critical temperatures from the maximum of $\tilde{\chi}$, and another with $N=164$ and B satisfying the following inequalities:

$$kT/N \ll B \ll kT_c \ . \tag{3}$$

This condition was imposed to be sure that the total magnetic moment keeps its orientation and that the local field of each spin is unaffected by the field B. With the last set of calculations, the temperature dependence of the magnetization was obtained. In Fig. 1 we present a typical $\tilde{\chi}$-versus-T curve of the first set of calculations obtained by Monte Carlo. The critical temperatures for the onset of ferromagnetism obtained are presented in Fig. 2 along with experimental data from Ododo[4] and references therein. The results are highly satisfactory and reproduce both the concentration dependence of the critical temperatures and the values themselves. It is interesting to note that the present model does not produce a real critical concentration but instead predicts that the critical temperatures decay exponentially as the concentration goes to zero. This behavior agrees with experimental data and with the behavior of *Pd*Fe. At higher concentrations we expect the model to begin failing because (a) we have neglected the direct exchange between neighboring iron atoms, and (b) positional short-range order may be present, as can be inferred from the neutron data of Ododo.[3]

The magnetization calculations are shown in Fig. 3. The most relevant feature is the fast decrease of the magnetization in comparison with a homogeneous system. We estimated the critical temperatures from this calculation using the inflexion points of the magnetization curves. The results agree within the statistical error with the values obtained in the first set of calculations.

NEUTRON SCATTERING CROSS SECTION

As we have already said in the Introduction, the disagreement between the calculated magnetization cloud $M(K)$ and the neutron scattering data[3] for dilute *Pt*Fe alloys suggest an important nonelastic contribution to such scattering. We calculated the neutron cross sections using the following formula:

$$T(\mathbf{K})=[0.27)^2c(1-c)N]^{-1}\frac{d\sigma}{d\Omega} \tag{4}$$

$$=|m(\mathbf{K})|^2\left[(\overline{\langle \mathbf{S}^{\perp}\rangle})^2+[c(1-c)N]^{-1}\sum_{ij}e^{i\mathbf{K}\cdot(\mathbf{r}_i-\mathbf{r}_j)}[\langle \mathbf{S}_i^{\perp}\cdot\mathbf{S}_j^{\perp}\rangle-(\overline{\langle \mathbf{S}^{\perp}\rangle})^2\right], \tag{5}$$

where $\mathbf{S}_i^{\perp}$ is the component of $\mathbf{S}_i$ perpendicular to $\mathbf{K}$, $\langle\ \rangle$ indicate thermal averages, the overhead bar indicates spatial averages, and $m(K)$ is the form factor of a magnetization cloud which is given directly by polarized-neutron scattering and is related to the $M(K)$ calculated in Ref. 2 by the following relation:

$$m(K)=\mu_{\mathrm{Fe}}f_{\mathrm{Fe}}+(1-c)f_{\mathrm{Pt}}[M(K)-\mu_{\mathrm{Fe}}] -c(M(0)-\mu_{\mathrm{Fe}})f_{\mathrm{Pt}} \ . \tag{6}$$

Here the f's are the atomic form factors.

The second term of Eq. (5) represents the thermal fluctuations. In deriving Eq. (5) we have assumed that the alloy is random, that magnetization clouds are independent, and that neutrons of any energy are measured.

The Monte Carlo calculations for $T(K)$ were made the same way as before but with a field **B** along the z axis assumed perpendicular to **K** and obeying the condition (3). The quantities to be calculated were $\langle S_i^z \rangle$, $\langle S_i \cdot S_j \rangle$, and $\langle S_i^z S_j^z \rangle$, from which we obtain the quantities appearing in Eq. (5) using the following relationships:

$$\langle \mathbf{S}_i^{\perp} \rangle = \langle S_i^z \rangle \hat{\mathbf{z}} , \tag{7}$$

$$\langle \mathbf{S}_i^{\perp} \cdot \mathbf{S}_j^{\perp} \rangle = \tfrac{1}{2} \langle S_i^z S_j^z \rangle + \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle . \tag{8}$$

The spherically averaged diffuse scattering cross section is then calculated as a function of wave vector K. We made the approximation of independently performing the spherical average of $m(K)$ and of the quantity in curly brackets in Eq. (5). The calculation was performed for a system of $N=200$ and a temperature of 4.2 K. The results are shown in Fig. 4 for 1.5 and 2.0 at. % Fe in Pt. The following features can be observed:

(a) The presence of a sharp peak, due to quasielastic scattering, which reproduces well the experimental neutron data below $K=0.25$ Å. This quasielastic scattering is produced by the magnetic fluctuations and correlations that become important for small K.

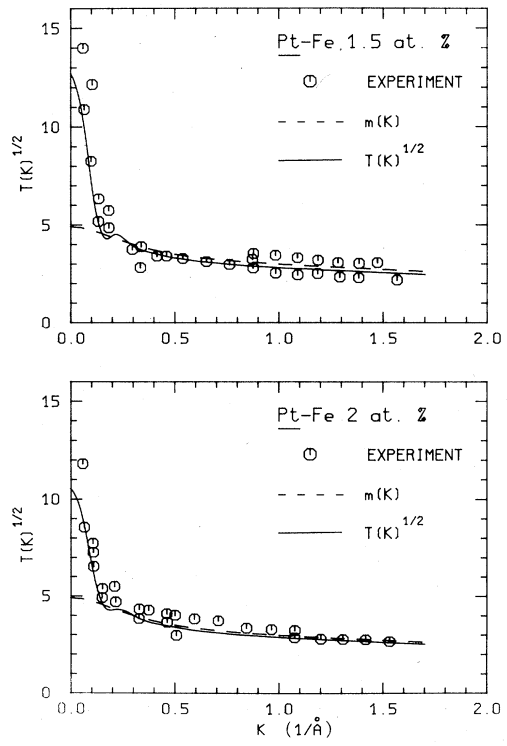

FIG. 4. Comparison of the experimental data of *Pt*Fe with calculated neutron scattering quantities using the model. $T(K)$ describes the unpolarized-neutron diffuse scattering and $m(K)$ represents the magnetization cloud.

(b) As the concentration increases the peak diminishes. This is a consequence of a decrease of magnetic fluctuations due to an increase of the critical temperature.

(c) For large values of K the scattering is identical to that produced by the magnetization cloud.

For the whole range of values of K, the calculated results agree with the experimental data, implying that the model used explains well the neutron scattering from these alloys at low concentrations.

At high concentrations the model should not apply as the clouds are considered to be independent in the calculations. Also, the model assumes that the spatial distribution of the atoms is totally random. In this case, however, due to the size difference between Pt and Fe atoms we can expect short-range order in this alloy. This order, of course, is not present in dilute alloys since the impurity atoms are almost isolated.

Recently, we applied a local-moment model[1] to dilute *Pd*Fe alloys without considering the quasielastic contribution to the scattering. The calculated results, however, agree quite well with magnetization and unpolarized-neutron data[5] in this case. This is surprising at first since Pd and Pt are, magnetically, very similar. To clarify this we repeated the calculation for *Pd*Fe with a concentration of 0.25 at. % Fe at a temperature of 4.2 K, which were also the experimental conditions. The results are presented in Fig. 5. The diffuse scattering $T(K)$ NOR (NOR denotes normalized) corresponds to a cross section normalized in the same fashion as the experimental data of Hicks *et al.*[5] They normalized their results so that the cross sections would agree, for large values of K, with the values of the cross section at a higher concentration (4 at. % Fe), to compensate for the lack of saturation at this temperature.

From the figure we notice the following:

(a) The diffuse cross section without normalization is below the experimental data, since it was calculated for a nonsaturated system.

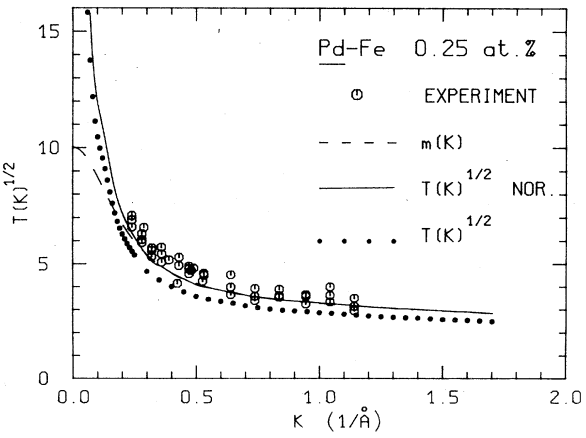

FIG. 5. Comparison of the calculated diffuse scattering cross section with experimental data for *Pd*Fe. $T(K)$, $T(K)$ NOR, and $m(K)$ are the calculated quantities using the model. $T(K)$ describes the unpolarized-neutron diffuse scattering, $T(K)$ NOR is the same $T(K)$ normalized as explained in the text, and $m(K)$ describes the magnetization cloud.

(b) There is a sharp quasielastic peak which does not contribute to the scattering for the K values for which the experiment was done ($K > 0.25$ Å). This is why our previous calculations for *Pd*Fe agree with experimental data.

CONCLUSIONS

The magnetic-environment model of giant-moment alloys successfully explains the magnetic properties of *Pt*Fe and *Pd*Fe at low temperatures, including the unpolarized-neutron scattering data. Although critical scattering is important, the size of the magnetization cloud of *Pd*Fe previously obtained from neutron data[5] was correct. In the case of *Pt*Fe no direct determination of the size of the cloud is possible from the neutron data,[3] although the cloud is quite large (a half-width of about 4 Å), as predicted by our model.[2]

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