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Abstract. – Analysis of polarized neutron scattering and magnetization measurements on dilute *Pd*Mn alloys using a magnetic *environment* model shows that both ferro- and antiferromagnetic interactions are present in these alloys. The results of the analysis allow us to calculate several magnetic properties of *Pd*Mn such as the exchange constant of ferromagnetism and the first neighbor antiferromagnetic moment perturbations. Critical temperatures were also calculated with this model using the Monte Carlo simulation method and the results compared with experimental data, showing a good agreement.

It is known that *Pd*Mn is a ferromagnet at dilute concentrations of the impurity, with an expected enhancement of the Pd moment. The work of Star *et al.* [1] (magnetization) and Cable and David [2] (neutron scattering) showed that Mn has giant moments of about 7.5 μ_B in Pd with approximately 4.0 μ_B located in Mn. It has also been shown that some antiferromagnetic Mn-Mn direct interactions are present in these materials [1].

We have developed a model [3] that has been applied successfully to other giant moment systems. In this paper we apply this model to *Pd*Mn taking into account antiferromagnetic interactions among Mn atoms.

In this model [3] the moment of a Pd atom at site n is given by

$$\mu_n = \chi_0 \, h_n, \tag{1}$$

where χ_0 is the nonenhanced susceptibility and h_n is a local field given by

$$h_n = b_n + J_{Pd} \sum_{\delta} \mu_{n+\delta} \left[1 + (\alpha - 1) \, P_{n+\delta}\right]. \tag{2}$$

Here b_n is the external field, J_{Pd} is the exchange constant between Pd atoms, αJ_{Pd} is the exchange constant between Mn and Pd and P_n is a site occupation operator.

With no impurities present we obtain from (1) and (2):

$$\chi = \frac{\chi_0}{1 - \Gamma}, \tag{3}$$

where $\Gamma = J_{Pd} \, Z_1 \, \chi_0$ and Z_1 is the first neighbors coordination number. The parameter Γ is the susceptibility enhancement parameter of Pd and was determined by Parra and Medina [4] as $\Gamma = 0.947 \pm 0.009$ from experimental neutron data.

A Fourier transformation of equation (1) gives us an expression for the magnetization cloud that can be related to the neutron scattering data:

$$M(K) = \left[\frac{\alpha}{\Phi_0 \left[1 - \Gamma F_1(K)\right]} + (1 - \alpha)\right] \mu_{Mn} \, f_{Mn}(K), \tag{4}$$

where $F_1(K)$ and Φ are the first neighbor shell structure factor and the moment perturbations on Pd respectively, and were determined by Medina and Parra.

To be able to use this equation we needed the values of μ_{Mn} for each concentration. These were obtained by fitting the neutron data of Cable and David with the following equations for polarized neutrons:

$$m(K) = \mu_{Mn} \, f_{Mn}(K) - \mu_{Pd} \, f_{Pd}(K), \qquad K \geq 1 \tag{5}$$

$$\bar{\mu} = \mu_{Mn} \, c + (1 - c) \, \mu_{Pd}. \tag{6}$$

In these expressions we used $f_{Mn}(K) = \exp\left(-0.069 \, K^2\right)$ and $f_{Pd}(K) = \exp\left(-0.1 \, K^2\right)$ which closely approximate the experimental form factors, and μ values obtained from magnetization data. The results for μ_{Mn} and μ_{Pd} are given in table I for each concentration. Star *et al.* [1] report several values for $M(0)$ in this concentration range. We used an average value, in this range, of $M(0) = 7.12 \; \mu_B$ / Mn. Using equation (4) we then calculate J_{PdMn} obtaining an average value of $J_{PdMn} = (48 \pm 7)$ K. Calculation of $M(K)$ using equation (4), should give us the experimental neutron $m(K)$. The calculated $M(K)$ values are compared in figure 1 with experimental values. This would be the expected $M(K)$ of polarized neutrons with only ferromagnetic interactions present. The comparison of calculated $M(K)$ values with the neutron experimental $m(K)$ clearly shows us that another kind of interaction is present in the neutron results. Atomic short range order (ASRO) has been found for Pd- 9.95 at. % Mn by Morgownik *et al.* [5]. However at very low concentrations of the impurity it is very improbable that ASRO would be found. It is expected, however, that antifer-

Table I. – *Values of the individual average moments* μ_{Mn} *and* μ_{Pd} *calculated from the neutron scattering data of Cable and David* [2]. *The values of* $a(R_1)$ *are the first neighbor antiferromagnetic moment perturbations.*

c (at. % Mn	μ_{Mn}	μ_{Pd}	$a(R_1)$
0.23	3.58	7.78×10^{-3}	-1.56×10^{-2}
0.46	4.14	1.10×10^{-2}	-1.73×10^{-2}
0.99	3.52	2.34×10^{-2}	-2.21×10^{-2}
1.99	3.62	3.04×10^{-2}	-3.06×10^{-2}
	± 0.07	$\pm 0.2 \times 10^{-3}$	$\pm 6.1 \times 10^{-3}$

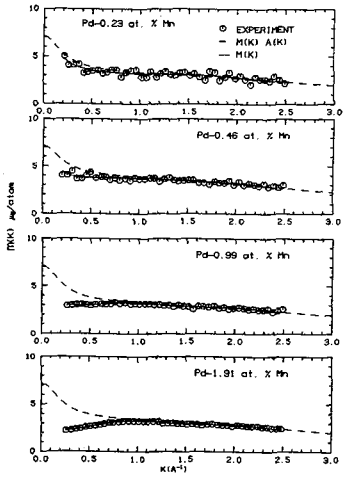

Fig. 1. – Experimental neutron scattering data $m(K)$ is compared with the model $M(K)$ and with a fitted $M(K)$ $A(K)$, which includes an antiferromagnetic interaction. The experimental data was taken from reference [2].

romagnetic Mn-Mn interactions would be present at all concentrations. We therefore analyzed the neutron scattering results with a function

$$m(K) = M(K)\ A(K), \tag{7}$$

where $M(K)$ is given by equation (4) and $A(K)$ is an antiferromagnetic interaction function that follows the Marshall model [6]:

$$A(K) = \sum_{j=0}^{n} Z_j\ a(R_j)\ \mathrm{e}^{iKR_j}, \tag{8}$$

and where we sum over the n near neighbor shells. A fitting of $m(K)$ with equations (7-8) is shown in figure 1. Values of the first neighbor, $a(R_1)$, parameters are presented in table I. These correspond antiferromagnetic moment disturbances and indicate an increasing importance of first neighbor antiferromagnetic interactions as the concentration of Mn is raised. The fitting also describe quite well the neutron scattering data.

The model [3] allows also the calculation of the critical temperatures of ferromagnetism. We have made Monte Carlo calculations for $c = 0.23$, 0.46, 0.99 and 1.91 at. % Mn, and considered a system of classical spins obeying the following Hamiltonian

$$H = (-1/2) \sum_{\substack{i,j \\ i \neq j}} J_{ij}(r_{ij})\ S_i.S_j, \tag{9}$$

where the values of J_{ij} were calculated in reference [3]. For each concentration we used samples of 100 spins with 2 000 Monte Carlo steps per spin. We calculated, for several temperatures, 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 M) and a quantity $\tilde{\chi}$ which is given by the fluctuation of the magnitude of the total moment and which is equal to χ for an infinite system. $\tilde{\chi}$ is given by

$$\tilde{\chi} = \frac{\left\langle (M - \langle M \rangle)^2 \right\rangle}{NkT}, \tag{10}$$

where N is the number of spins. Critical temperatures were obtained from the maximum of $\tilde{\chi}$ against temperature. To compare the calculated critical temperatures with the experimental ones (in degrees Kelvin) we must multiply the calculated T_c's by a factor $J_0 = J_{\mathrm{Pd}}(\alpha\mu_{\mathrm{Mn}})^2$. The factor comes from equation (4) (see Ref. [3]). Notice however that we are really analyzing the neutron scattering $m(K)$ with a function $M(K)\,A(K)$ and therefore our new factor J_0 must be:

$$J_0 = J_{\mathrm{Pd}}(\alpha\mu_{\mathrm{Mn}}\ A(0))^2, \tag{11}$$

where $A(0)$ is the calculated value of $A(K)$ at $K = 0$. In this way we are taking into account the assumed antiferromagnetic interactions. The T_c's obtained in this way are compared with experimental values in figure 2. We observe that the calculated values agree, in general, with experimental T_c's.

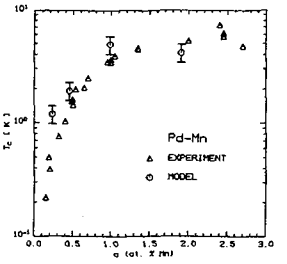

Fig. 2. – Critical temperatures of ferromagnetism, taking into account Mn antiferromagnetic interactions, are compared with experimental data from reference [1] and other references therein.

In this paper we presented an analysis of PdMn data with a magnetic environment model. In this model, for very low concentrations ferromagnetism dominates making possible the formation of giant moments. As the Mn concentration is increased the probabiliy of a Mn atom as nearest neighbor of another Mn increases. This introduces an antiparallel coupling of Mn nearest neighbors creating an antiferromagnetic exchange attached to the long range ferromagnetic order.

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