INELASTIC NEUTRON SCATTERING ON THE SPIN GLASS : PdMn 10 at.%*

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Résumé.— Par la contribution inélastique de la diffusion de neutrons à un verre de spin Pd-Mn on a déterminé la répartition de probabilités d'énergies de couplage P(E) qui paraît être en bon accord avec les résultats d'une simulation numérique. La chaleur spécifique, calculée selon cette répartition, est conforme aux résultats expérimentaux.

Abstract.— From the inelastic contribution to the neutron scattering on a PdMn spin glass the probability distribution P(E) of exchange energies was determined which was in good agreement with computer simulation results. From this P(E), the specific heat could be calculated with close conformity to experiment.

The random molecular field model as developed by Marshall /1/ and by Klein and Brout /2/ offers a simple method with which to theoretically investigate the spin glass freezing process. Several analytical expressions for the molecular field distribution P(H) have been proposed depending upon the concentration /3/. However, for very small exchange fields (H → 0), discrepancies exist between the distribution function obtained from the above mentioned spin glass theories and that resulting from a computer simulation calculation /4/. Details of the complete P(H) distribution usually can only indirectly be deduced from experiments because of the different averaging procedures involved in the various measurements.

In this paper we suggest that inelastic neutron scattering can directly give the probability distribution of exchange fields P(H) from the excitation spectrum of single spins in the spin glass ground state. We have performed neutron scattering experiments on the spin glass alloy PdMn 10 at.% at T = 4.2 K < T_f = 9 K. For this system the complex magnetic interactions - producing the spin glass state - have been extensively studied /5/. The measurements have been carried out on a triple axis spectrometer at the Petten HFR reactor with incident energy E_i = 13.5 meV while the sample (dimensions 27 x 27 x 9 mm) was kept in liquid helium. In order to correct for background and nuclear scattering, a pure Pd sample with the same dimensions was measured under identical conditions.

A 2 mm thick V plate was used for calibration and determination of spectrometer resolution. Figure 1 shows typical scattering results-corrected for background-from PdMn 10 at.% for Q = 0.8 Å⁻¹. The elastic peak contains a large incoherent nuclear contribution and the quasi-paramagnetic scattering from the randomly frozen spins. At the energy loss side a break inelastic contribution is clearly observed. The intensity of this contribution decreases with increasing scattering vector Q approximately as a 3-d form factor, indicating that the scattering mechanism is of single spin origin.
Separate experiments with high resolution \((E_0 = 5 \text{ meV}, \text{FWHM}=0.23 \text{ meV})\) showed no broadening of the elastic line compared to the spectrometer resolution. This enabled us to separate the inelastic contribution from the total scattering by fitting the \(\text{PdMn}\) elastic peak to a Gaussian curve with the spectrometer resolution halfwidth (FWHM = 1 meV) — see the solid line in figure 1. The magnetic inelastic contribution is shown in greater detail in figure 2 by the dots. The shaded area represents the overlap with the elastic line, which causes the large error bars in this region. Nevertheless, an asymmetric energy spectrum is obtained which reflects the internal magnetic energy distribution \(P(E = \mu \text{H})\) of the Mn spins in the spin glass ground state. The origin of a distribution is found in the random interactions with the neighbouring magnetic moments.

The magnetic energy distribution can also be obtained from a computer simulation of the \(\text{PdMn}\) 10 at.% alloy with an appropriate distance dependence of the interaction strength /5/. We have carried out such calculations for an Ising \(S = \frac{1}{2}\) system (fcc lattice with 109 spins) and minimized the energy of the system by the Monte Carlo method. The energy distribution is obtained as the average over 44 configurations. The results of this calculation are illustrated in figure 2 by the histogram. Remarkably good agreement is found with the neutron data, supplying further evidence for our interpretation of the scattering data. As an additional check we have calculated the magnetic specific heat using the measured energy distribution and compared it with the experimental results for \(\text{PdMn}\) as obtained by Zweers at al /6/ shown in figure 3. At low temperatures good agreement is found between the calculated and experimental specific heat. At higher temperatures, \(T > T_c\), deviations occur since the temperature dependence of the energy distribution has not been taken into account.

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**Fig. 2**: Expanded scale of the inelastic scattering contribution. The shaded area is the elastic peak. The histogram represents the result of the computer simulation calculation.

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**Fig. 3**: Magnetic specific heat of \(\text{PdMn}\) 10 at.%: (o) experimental data, solid line: Calculated specific heat based on measured \(P(E)\)

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**References**

/1/ Marshall, W., Phys. Rev. 118 (1960) 1520
/2/ Klein, M.W. and Brout, R., Phys. Rev. 132 (1963) 2412