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MAGNETIC EXCITATIONS IN Ni-DOPED KMnF₃

T. M. HOLDEN, R. A. COWLEY, W. J. L. BUYERS AND E. C. SVENSSON

Chalk River Nuclear Laboratories
Atomic Energy of Canada Limited
Chalk River, Ontario, Canada

and

R. H. W. STEVENSON
Aberdeen University, Scotland

Résumé. — Les excitations magnétiques dans un cristal de KMn₀.₉Ni₀.₀F₃ ont été étudiées à 15 °K, par diffusion inélastique de neutrons. Les fréquences des ondes de spin acoustiques ne sont que peu déplacées des valeurs correspondantes pour KMnF₃ pur. Près des frontières de zones, les modes acoustiques se confondent avec une bande de modes magnétiques ayant des fréquences dans la bande 2.05-2.30 THz. Ces derniers sont observés dans des zones de Brillouin contenant les points du réseau réciproque magnétique et nucléaire et sont associés avec des excitations localisées sur les voisins Mn d'une impureté Ni. Un mode magnétique est aussi observé à 7.7 ± 0.3 THz correspondant à une excitation localisée sur une impureté Ni. Des calculs de perturbation des modes acoustiques et les énergies des modes d'impureté, calculés selon des techniques de fonctions de Green, donnent un agrément qualitatif avec les observations.

Abstract. — The magnetic excitations in a crystal of KMn₀.₉Ni₀.₀F₃ have been studied at 15 °K by means of neutron inelastic scattering. The frequencies of the acoustic spin waves are only slightly shifted from the corresponding values for pure KMnF₃. Near the zone boundaries the acoustic modes merge with a band of magnetic modes having frequencies in the range 2.05-2.30 THz. The latter are observed in Brillouin zones containing nuclear and magnetic reciprocal lattice points and are associated with excitations localized on the Mn neighbours of a Ni impurity. A magnetic mode is also observed at 7.7 ± 0.3 THz which corresponds to an excitation localized on a Ni impurity. Calculations of the perturbation of the acoustic modes and the energies of the impurity modes carried out with Green-function techniques, give qualitative agreement with the observations.

Experiment. — Neutron inelastic scattering measurements have been made of the magnetic excitations in antiferromagnetic nickel-doped KMnF₃. Since Ni²⁺ has spin 1 compared with 5/2 for Mn²⁺, and since the exchange between nickel and manganese differs from that between host ions, the magnetic excitations will be perturbed by the nickel impurities and local [1] and/or resonant [2] impurity modes may occur.

The measurements were carried out with a triple-axis crystal spectrometer at the NRU reactor. The constant-momentum transfer (constant-Q) technique was used to measure the scattering for momentum transfers in zones containing magnetic and nuclear reciprocal-lattice points. Magnetic modes were observed at several frequencies (Fig. 1) and could be divided into local, shell, and band modes. The local mode was observed at a frequency of 7.7 ± 0.3 THz (Fig. 1d) which was independent of Q. This mode (s₈) corresponds to a spin deviation that is essentially localized on the nickel impurity.

The shell modes (s₈, p, d modes) were observed in the frequency range 2.05-2.3 THz and are associated with spin deviations on the shell of manganese ions that are nearest neighbours to a nickel impurity ion. The shell modes are well separated (Fig. 1a and 1b) from the band modes except near zone boundaries where the two excitations merge and appear as a single neutron group. The band modes, which correspond to modes of the host crystal perturbed by the impurities, are strong in magnetic zones but weak in nuclear zones. By contrast, the shell modes have comparable intensity in both zones. We have confirmed that all three types of excitation are of magnetic character by observing that they are absent above the Néel temperature (Fig. 1c and 1d).

The dispersion curves for the shell and band modes for the [00l] and [l0l] directions are shown in figure 2. In general, the band modes differ little from those for pure KMnF₃ as determined by Pickart et al. [3] by neutron scattering which are shown as the solid line in figure 2. There is a significant difference near the zone center (ζ = 0); however, the ζ = 0 frequency of Pickart et al. is much higher than is indicated by AFMR measurements [4]. The shell modes do not exhibit any marked dispersion, but there is some

![Graph](image-url)
MAGNETIC EXCITATIONS IN Ni-DOPED KMnF$_3$

As was found for cobalt-doped KMnF$_3$ [8] the geometric mean relationship

$$J_{J_1-J_n} = (J_{J_1-J_n} \times J_{J_n-J_m})^{1/2} = 0.266 \text{ THz}$$

reasonably accurately predicts the magnitude of the impurity-host exchange. The values of $J_{J_1-J_n}$ and $J_{J_n-J_m}$ were taken from the results of Pickart et al. [3] and Lines [9].

In the Ising model the $s_1$, $p$ and $d$ modes are degenerate with a frequency of

$$25 J_{J_1-J_n} + 2 J_{J_1-J_n} = 2.42 \text{ THz}$$

which is $\approx 0.13$ THz above the band. Since the experimental frequencies lie in the range 2.05-2.30 THz, the Ising model is again seen to give a reasonable description of the results. Although the maximum frequency of the band modes is only approximately known, the occurrence of the shell modes over a large region of reciprocal space with about equal intensity suggests that they are indeed local, in agreement with the Ising model.

Green-function theory. — The properties of the magnetic excitations in KMn$_{0.97}$Ni$_{0.03}$F$_3$ have been calculated using Green-function techniques following the method of Elliott and Taylor [10]. Three shell modes with different structure factors are found at 0.05 THz($s_1$), 0.07 THz($p$) and 0.08 THz($d$) above the top of the band, in better agreement with experiment than the Ising model. A calculation by Parkinson [11] gave very similar shell mode frequencies (0.10 THz and 0.11 THz above the top of the band for $p$ and $d$ modes). From our theory we have also obtained widths and shifts ($< 0.02$ THz) for the band modes which are consistent with experiment where comparison is possible.

Summary. — The local, shell and band modes in KMn$_{0.97}$Ni$_{0.03}$F$_3$ have been studied by neutron inelastic scattering techniques. The shell modes are localized in this crystal because $J_S$ for the impurity-host interaction is $\approx 40$% greater than $J_S$ for the host. The results are in good agreement with optical measurements which, unlike neutron scattering, do not determine the shell mode frequency directly. Our experimental results are described qualitatively by an Ising model, and somewhat more fully by a Green-function theory.

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