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THE MAGNETIC FORM FACTOR OF TERBIUM (*)

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Abstract. — The magnetic form factor of terbium has been measured with polarized neutrons using single crystals held in an applied magnetic field of 24 kOe at room temperature. Except for the low angle reflections the experimental points lie on a smooth curve approximately 14 % below the theoretical form factor. These results suggest that the Hartree-Fock 4-f electron wavefunctions are too contracted in real space.

I. Introduction. — The magnetic form factor of terbium in the ordered magnetic state at 4.2 °K has been measured with polarized neutrons [1]. The magnetic scattering length \( p \) is defined as

\[ p = 0.27 \times \mu \times f(\kappa) \times 10^{-12} \text{ cm}, \]

where \( \mu \) is the ordered moment in Bohr magnetons, and \( f(\kappa) \) is the form factor. For terbium in the ordered state the moment is \( 9 \mu_B \) so that at low scattering angles \( p \) is larger than the nuclear scattering length, \( b \). Under these conditions the experimental difficulties associated with extinction become severe, and, in [1], no accurate values were reported for the low angle reflections. At high angles the experimental form factor for terbium was found to be essentially a smooth curve, indicating that the crystal field is isotropic within the basal plane.

In view of the results obtained in a polarized-neutron study of thulium [2], we have remeasured the terbium form factor under different experimental conditions so as to obtain accurate values of \( f(\kappa) \) at low angles. By examining different orientations in the paramagnetic state we confirm that the crystal field interactions are isotropic within the basal plane.

II. Results. — The single crystals for these studies were kindly provided by Professor F. H. Spedding. The crystals were cut in the shape of parallelopipeds and the field was applied along the long axes, either \( <10.0> \) or \( <11.0> \). Two crystals of each orientation, \( b \) and \( a \), respectively, were studied. In order to minimize extinction the neutron wavelength was 0.85 Å, and the neutron path lengths never exceeded 1.5 mm. The crystals were also mechanically worked to increase the mosaic spread. The applied magnetic fields varied between 21 and 26 kOe, depending on the length of the sample (6 to 9 mm). In each case the field was homogeneous, and the absolute field strength was measured with an accuracy of 1.5 %. The experiments were performed at room temperature. A coherent scattering length of 0.76 \( \times 10^{-12} \) cm was used to normalize the magnetic scattering amplitudes.

For these values of the field and temperature the magnetization measurements [3] indicate that the Curie-Weiss law is obeyed, and the value of the induced moment is \( \sim 0.88 \mu_B \), depending on the exact value of \( H \). The magnetic form factor is calculated by taking account of the population of the various \( M_s \) states. The calculation reduces to a very simple form if the Curie-Weiss law is strictly valid [4]. For terbium the form factor associated with the induced moment in the paramagnetic state is given by

\[ f(\kappa) = <j_0> + 0.370 37 <j_2>. \]

The functions \( <j_0> \) and \( <j_2> \) are directly related to the radial wavefunction of the 4f electrons, and have been tabulated by Blume, et al. [5]. The experimental points for both the \( a \) and \( b \)-axes crystals are shown in figure 1, together with the theoretical form factor.

III. Discussion. — Within experimental error the points for the \( a \) and \( b \) orientations fall on the same smooth curve, indicating that the crystal field is isotropic within the basal plane. At high values of \( \sin \theta/\lambda \) the points lie on a smooth curve given by

\[ 0.86 \times f_{\text{theory}}, \]

in agreement with the previous results for terbium [1]. At low angles the discrepancy between theory and experiment is much less, and this result is very similar to that found in thulium [2]. Since the normalization, i.e., \( f(0) = 1 \), depends on the nuclear scattering length and the magnetic field, this factor could be wrong by possibly 3-4 %. However, independently of the norma-
The experimental (points) and theoretical (solid line) magnetic form factors for terbium in the paramagnetic state. The broken line is a smooth curve drawn through the experimental points.

A similar discrepancy in thulium was explained by postulating that a large 5\textit{d} conduction-electron polarization contributes to the magnetization density. Therefore the discrepancy between the experimental and theoretical magnetic form factors for terbium probably cannot be explained in terms of a large 5\textit{d} conduction-electron contribution to the magnetization density. A more likely interpretation of the discrepancies for both terbium and thulium is that the theoretical 4\textit{f} wavefunctions are too contracted. Of course, this interpretation is not incompatible with an effective contribution from the 5\textit{d} shell, since these electrons are more extended than those in the 4\textit{f} shell.

A comparison between the calculated and experimental values for the $<r^6>$ crystal-field integrals for the heavy rare-earth metals [6] also provides further evidence that the theoretical wavefunctions are too contracted. The wavefunctions used in these comparisons, and also in calculating the $<j_i>$ integrals for the magnetic form factor, are those given by Freeman and Watson [7]. In an attempt to resolve the discrepancies between theory and experiment we have examined more recent 4\textit{f} wavefunctions [8, 9], but they differ very little from those in [7], suggesting that the Hartree-Fock wavefunctions for the tripositive ions are a poor approximation to the metallic state.

References