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Determination of exchange and crystal field effects in Sm alloys by polarized neutron diffraction

J. X. Boucherle (*), D. Givord (♦+), J. Laforest (*), J. Schweizer (♦+) and F. Tasset (+)

(*) DRF/DN, C.E.N.G., 85X 38041 Grenoble Cedex, France
(♦) Laboratoire Louis-Néel, CNRS, 166X 38042 Grenoble Cedex, France
(+ ) Institut Laue-Langevin, 156X 38042 Grenoble, France

Résumé. — Par diffraction de neutrons polarisés à λ = 0.5 Å, nous avons mesuré le facteur de forme du samarium dans SmAl₃ et SmCo₅. Nous en avons déduit les valeurs des interactions d’échange et des paramètres de champ cristallin. Ces résultats montrent que la polarisation des électrons de conduction dans SmAl₃ est forte et que SmCo₅ est encore ferromagnétique à 300 K.

Abstract. — The form factor of samarium in SmAl₃ and SmCo₅ has been measured at λ = 0.5 Å by the polarized neutron technique. This has enabled us to deduce the values of the exchange interaction and the crystal field parameters. The results show that there is a large conduction electron polarization in SmAl₃ and that SmCo₅ is still ferromagnetic at 300 K.

1. Introduction. — The peculiar properties of Sm result from the proximity of the excited multiplets to the ground state \( J = \frac{5}{2} \). Based on that consideration Van Vleck has given an account of the behaviour of the low temperature magnetic susceptibility. Furthermore the need for C.E.F. sixth order terms to explain the physical properties is direct evidence of the influence of excited multiplets.

Recently, results concerning R.E. alloys have been well explained in terms of exchange and C.E.F. [1, 2]. For samarium alloys, bulk magnetization analysis is made difficult by the weakness of the magnetic moment of Sm. Due to the extremely high true absorption cross-section of natural samarium for 1 Å neutrons, only a few neutron studies have been made [3, 4] and, for these, non-absorbing Sm isotopes were used. Taking advantage of the hot source of I.L.L. we have performed measurements by polarized neutron diffraction on SmAl₃ and SmCo₅ single crystals. In effect, in the range λ = 0.5 Å to 0.34 Å the absorption of natural Sm is less than 200 barns.

2. Experimental. — The polarized neutron spectrometer D5 was used at \( \lambda = 0.42 \) Å and 0.50 Å. In the cubic Laves phase compound SmAl₃ the easy magnetization axis [111] was aligned along a 1.65 tesla vertical magnetic field. At 4.2 K classical flipping ratios of Bragg reflections in the zero layer were measured up to \( \sin \theta/\lambda = 1.64 \) Å⁻¹. Under the same experimental conditions the bulk magnetization was 0.23 (1) \( \mu_B/\text{Sm} \). SmCo₅ crystallizes in the hexagonal CaCu₅ type structure, the crystal was oriented with the easy c axis parallel to a 1.65 tesla vertical applied field. Zero layer reflections and some important 1st order ones were collected at 4.2 and 300 K up to \( \sin \theta/\lambda = 1.38 \) Å⁻¹.

Due to the proximity of resonant absorption peaks, the Sm scattering length \( b_{\text{Sm}} \) is wavelength dependent. In both crystals \( b_{\text{Sm}} \) and the nuclear structure were refined using a combination of integrated intensities and flipping ratios measurements.

3. Results and analysis. — The Sm form factor was calculated using the tensor operator method [5], the radial distribution being taken from relativistic calculations [6]. In SmAl₃, since the magnetization is along the 3-fold axis and according to the value of the exchange field \( (\mu_B H_{\text{ex}}/k = 50 \text{ K}) \) [7], the ground wave function involves terms of the form \( |J, \frac{5}{2} - 3n\rangle \) (\( n \) integer). By comparing experimental and calculated form factors (figure 1) we find that only the following terms are significant:

\[
\psi = 0.958 \left| \frac{5}{2}, \frac{5}{2} \right> - 0.264 \left| \frac{5}{2}, -\frac{1}{2} \right> - 0.085 \left| \frac{3}{2}, \frac{3}{2} \right> + 0.075 \left| \frac{3}{2}, -\frac{1}{2} \right> + \cdots
\]

The Sm magnetic moment deduced is only 0.44 \( \mu_B \) which indicates a conduction electron polarization of 0.21 \( \mu_B \). This value is large compared to the 0.15 \( \mu_B \) expected from a comparison with GdAl₃ results ; it is in line with those obtained in other RAl₃ alloys [8, 9].

In a cubic environment the crystal field is described by 2 parameters \( A_4 \left< r^4 \right> \) and \( A_6 \left< r^6 \right> \). Values compatible with the experimental wave function are...
DETERMINATION OF EXCHANGE AND CRYSTAL FIELD EFFECTS IN \( \text{Sm} \)

shown by the shaded area in the insert of figure 1. They are in fair agreement with those previously reported [7] as well as with a scaling law [2].

![Diagram](image1.png)

**Fig. 1.** — Observed (●) and calculated (○) form factor of \( \text{Sm}^{3+} \) in \( \text{SmAl}_2 \). The insert gives a representation of the ground state moment as a function of 4th and 6th order C.E.F. parameters [7]. The values obtained from form factor measurement (shaded area) are compared to those provided in [7] (●) and those calculated by the scaling law (□).

The measured flipping ratios show that \( \text{SmCo}_5 \) is ferromagnetic. On each reflection at 4.2 and 300 K the Sm magnetic amplitude (figure 2) was obtained by subtracting the strong cobalt contribution deduced from YCo\(_2\) [10]. At 4.2 K the ground wave function \( \psi_G \) involves terms of the form \( |J, \frac{1}{2}, \frac{3}{2} > \), neglecting the \( V_6 \) crystal field term. From the experiment we deduced:

\[
\psi_G = 0.978 | J, \frac{1}{2}, \frac{3}{2} > - 0.205 | J, \frac{1}{2}, \frac{1}{2} > + 0.038 | J, \frac{1}{2}, \frac{3}{2} > .
\]

Besides exchange interactions, mainly due to Co atoms, the Hamiltonian depends on 3 C.E.F. parameters \( A_2^0 \langle r^2 \rangle, A_4^0 \langle r^4 \rangle, A_6^0 \langle r^6 \rangle \). From \( \psi_G \) and by fitting the form factor at 300 K, where the population of excited levels is large, we have obtained

\[
\mu_B H_{\text{ex}}/k = 175 \pm 25 \text{ K},
\]

\[
A_2^0 \langle r^2 \rangle = -200 \pm 50 \text{ K},
\]

\[
A_4^0 \langle r^4 \rangle = 0 \pm 50 \text{ K},
\]

\[
A_6^0 \langle r^6 \rangle = 50 \pm 50 \text{ K}.
\]

![Diagram](image2.png)

**Fig. 2.** — Form factor of \( \text{Sm}^{3+} \) in \( \text{SmCo}_5 \) at 4.2 and 300 K. (○): zero layer reflections; (●): first layer reflections. The solid lines represent the calculated form factor.

These values are in good agreement with those reported in reference [11] and in reference [12]. Such values give a good description of the temperature dependance of the anisotropy: the large R-Co interactions at 300 K lead to the strong anisotropy responsible for the permanent magnet properties of \( \text{SmCo}_5 \). From these results it appears that \( \text{SmCo}_5 \) is still ferromagnetic at 300 K, the Sm moment cross over being calculated to take place at 350 K.

4. Conclusion. — On two Sm alloys, \( \text{SmAl}_2 \) and \( \text{SmCo}_5 \), where respectively the C.E.F. and the exchange interactions are dominant, we have shown polarized neutron diffraction technique to be specially suitable for magnetic investigations since the interpretation of bulk magnetic measurements is made difficult by the weakness of the Sm moment.
References