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Neutron diffraction study of $NdScO_3$ below 1 K Magnetic structure and hyperfine enhanced polarization of Nd

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Abstract

The ordered magnetic structure of the $NdScO_3$ perovskite has been studied below its phase transition ($T_c = 0.953$ K) by means of powder neutron diffraction. Its configuration is $g_y a_x$ with a magnetic moment of $(2.1 \pm 0.1)\mu_B$. The thermal evolution of the integrated intensity of some magnetic peaks shows a strong enhancement below 200 mK, interpreted as due to the hyperfine polarization of the ^{143}Nd and ^{145}Nd nuclear moments.

Keywords: Magnetic order; Nuclear polarization; Perovskite compounds; Powder diffraction

The $NdScO_3$ belongs to a family of orthorhombically distorted perovskites (space group Pbnm, $Z = 4$) [1]. Previous specific heat measurements showed a sharp peak at $T_c = 0.953$ K, interpreted as the onset of magnetic order of Nd^{3+} ions. The aim of this work is to determine the $NdScO_3$ magnetic structure below 1 K.

At low temperatures, due to the hyperfine electronic field, the incoherent scattering lengths of ^{143}Nd and ^{145}Nd become partially coherent, increasing the intensity of the magnetic reflections. This effect has been observed in $NdGaO_3$ [2], Nd_2CuO_4 [3], and $NdFeO_3$ [4]. We have searched for the same effect in $NdScO_3$ below 200 mK.

Powder neutron diffractograms were taken in the ILL (D1B) with $\lambda = 2.52$ Å, 20 mK $< T < 1.2$ K, using a ^3He-^4He dilution refrigerator. The $\lambda/2$ radiation was reduced by a pyrolitic graphite filter. Data were analysed at 500 mK with the FULLPROF [5] program. At other temperatures the integrated intensities of selected peaks were derived from the diffractograms. The atom coordinates have been refined using the difractogram taken at 5 K, used also to determine spurious peaks and background due to the cryostat.

Fig. 1 shows the observed and calculated patterns. Table 1 shows the refined parameters. The presence of the (0 0 1), (0 1 1), (1 0 1) magnetic peaks can be interpreted as corresponding to the $g_y a_x$ (Γ_8) configuration in the Bertaut's notation [6] with a magnetic moment of $\mu = 2.07(13)\mu_B$. The structure is similar to that of $NdInO_3$ (see Fig. 2(b) in Ref. [7]) and quite different from those of the chemically isostructural $NdGaO_3$ and $NdCoO_3$, (c_z mode, $\mu \cong 1\mu_B$) [7].

Besides, below 200 mK the integrated intensity of the (0 0 1), (0 1 1), (1 0 1), (1 2 1) + (0 1 3) and (1 0 3) + (2 1 1) peaks increases strongly due to hyperfine polarization enhancement.

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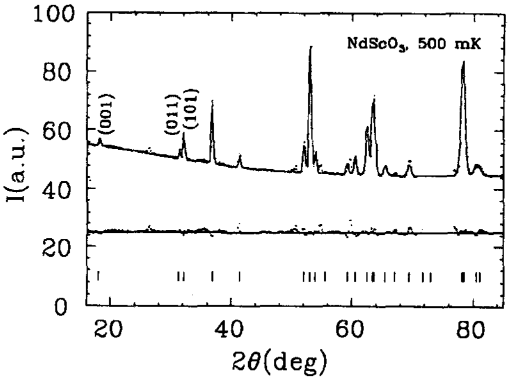

Fig. 1. Neutron powder diffraction pattern of $NdScO_3$ at 500 mK. The Al (1 1 1) and (2 0 0) reflections of the sample holder and cryostat produce bands near $2\theta = 65°$ and 77° and weak ones near 31° and 36° due to the harmonic $\lambda/2$.

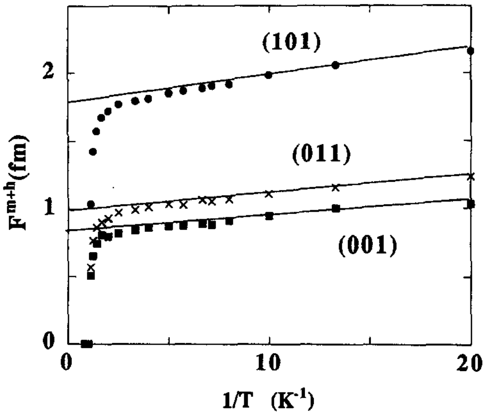

Fig. 2. Thermal evolution of $|F^{h+m}|$. The scale factor has been obtained from the nuclear/magnetic factors at 500 mK.

Table 1
Refined structural parameters at $T = 500$ mK. The standard deviation is in parenthesis. s. g. Pbnm, $Z = 4$, $a = 5.555(1)$ Å, $b = 5.744(1)$ Å, $c = 7.972(2)$ Å, $R_{wp} = 4.3\%$, $R_{Bragg} = 4.7\%$

	x	y	z
O1	0.113(3)	0.527(5)	1/4
O2	0.686(2)	0.282(2)	0.089(3)
Sc	1/2	0	0
Nd	0.001(4)	0.024(3)	1/4
$\mu(\mu_B)$	0.89(12)	1.87(13)	0

The magnetic + hyperfine intensity is proportional to the square of the structure factor vector $\boldsymbol{F}^{m+h}(\tau)$ given by [4]

$$\boldsymbol{F}^{m+h}(\tau) = \sum_r \left[-\alpha f_r(\tau)\langle \hat{\boldsymbol{M}}_{r\perp}\rangle + \frac{b_{ri}}{\sqrt{I_r(I_r+1)}}\langle \hat{\boldsymbol{I}}_r\rangle \right] \times \exp(\mathrm{i}\tau\cdot\boldsymbol{r}). \quad (1)$$

$f_r(\tau)$ is the magnetic form factor of the atom at $\boldsymbol{r}(Nd^{3+})$, $\langle \hat{\boldsymbol{M}}_{r\perp}\rangle$ is the thermal average of the component perpendicular to τ of the electronic magnetic moment vector of the atom at $\boldsymbol{r}$, $\langle \hat{\boldsymbol{I}}_r\rangle$ the average of the nuclear spin and b_{ri} the incoherent scattering length of the atom at $\boldsymbol{r}$. The hyperfine term in the square bracket in Eq. (1) can be approximated by the high temperature limit of the Brillouin function under a hyperfine field $\boldsymbol{B}_{hf}$; i.e. $b_{eff}\,\mu_N B_{hf}/k_B T$ being $b_{eff} = (5.3 \pm 0.7) \times 10^{-15}$ m the isotopic average for ^{143}Nd and ^{145}Nd scatterers [4]. The fit of $|\boldsymbol{F}^{m+h}(\tau)|$ allows to determine the hyperfine field $\boldsymbol{B}_{hf}$. Fig. 2 shows a plot of $|\boldsymbol{F}^{m+h}(\tau)|$ which is linear with $1/T$ at low temperatures. $\boldsymbol{B}_{hf}$ deduced from the slope (in the limit $1/T \to \infty$) of the plot is $(B_{hf})_x = 50(5)$ T and $(B_{hf})_y = 90(15)$ T. $\boldsymbol{B}_{hf} = 110(20)$ T, which is similar to the field in other Nd compounds such as $NdGaO_3$, $NdFeO_3$ or Nd_2CuO_4.

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