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Neutron diffraction study of the magnetic ordered Nd^{3+} in $NdCoO_3$ and $NdInO_3$ below 1 K

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Abstract

The ordered magnetic structure of the $NdCoO_3$ and $NdInO_3$ perovskites has been studied, below 1 K, by means of powder neutron diffraction. $NdCoO_3$ compound orders in the c_z (Γ_1) magnetic configuration while the isostructural $NdInO_3$ orders in $g_y a_x$ (Γ_8). At $T = 250$ and 280 mK, the saturation Nd magnetic moments $\mu_{Nd} = (1.4 \pm 0.1)\mu_B$ and $(2.9 \pm 0.2)\mu_B$ for the Co and In compounds, respectively, have been deduced. The different order configurations are discussed in terms of the interatomic distances and Nd–O–Nd angles.

Keywords: Magnetic order; Perovskite compounds; Powder diffraction

We have shown that Nd–Nd interactions are able to induce magnetic ordering at temperatures near 1 K in $NdMO_3$ with M = Ga, Co, Fe and Ni [1, 2]. The $NdMO_3$ perovskites have the Pbnm orthorhombic structure, with four distorted perovskite pseudocells in the crystallographic unit cell. Recent powder diffraction experiments have shown that the $NdGaO_3$ compound ordered below T_N in the c_z configuration [3] (in Bertaut's notation [4]). The Nd magnetic moment was determined to be $\mu_{Nd} = 1.1(2)\mu_B$.

To study the Nd–Nd superexchange interaction dependence on interatomic distances and angles, the isostructural compounds $NdCoO_3$ and $NdInO_3$ have been measured, since Co^{3+} and In^{3+}, which belong to the same period and group, respectively, as Ga^{3+}, are non-magnetic at low temperatures. $NdCoO_3$ orders at $T_N = 1.20(1)$ K [2] and $NdInO_3$ at 1.185(2) K [5].

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The neutron powder diffraction patterns were recorded in the ILL (D1B) and BENSC (E4) diffractometers with incident wavelength of $\lambda = 2.52$ and 2.40 Å, respectively, at 250 mK $< T <$ 1.4 K using a ^{3}He–^{4}He dilution refrigerator. The data were analysed with the Rielveld program FULLPROF [6].

In the $NdCoO_3$ pattern, the presence of the magnetic pairs (1 0 0) + (0 1 0) and (1 0 2) + (0 1 2), which cannot be resolved, and their intensity ratio are compatible with the Nd sublattice ordering in a c_z mode with a moment of $(1.4 \pm 0.1)\mu_B$ at $T = 250$ mK (Fig. (1a)). This configuration and magnetic moment are similar to these in the Ga compound [3].

In contrast, in the $NdInO_3$ pattern at $T =$ 280 mK, the only magnetic peaks are the well separated (0 1 1) + (1 0 1) pair, characterising g configuration and the (0 0 1) peak, characteristic of a configuration. The integrated intensity ratio of the (0 1 1) and (1 0 1) peaks is $r = 0.353(17)$, compatible with the g_y mode prediction, $r = 0.354$. From the unique (0 0 1) peak it is impossible to determine

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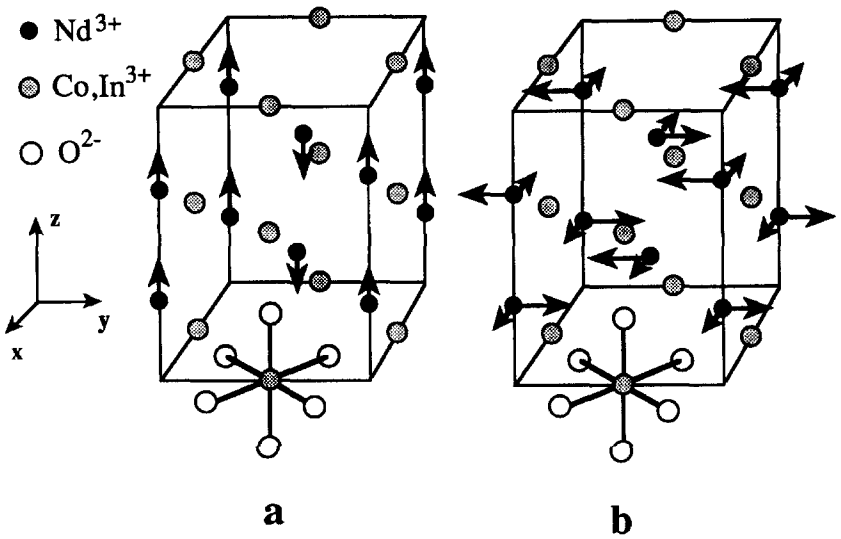

Fig. 1. Magnetic structures of (a) $NdCoO_3$ at 250 mK and (b) $NdInO_3$ at 280 mK.

the direction of the magnetic moments for the a component but a_x belongs to the same irreducible representation (Γ_8) as the g_y component. So the simplest assumption for the magnetic structure is the $g_y a_x$ combination, although it is not the only one mathematically compatible with the experimental data. The magnetic moment $(2.9 \pm 0.2)\mu_B$, is more than twice larger than those of the Ga and Co isostructural compounds . The magnetic structure is depicted in Fig. 1(b) and the final fitting parameters are listed in Table 1.

The c_z magnetic structure of the Ga and Co compounds may be described as a stack of antiferromagnetically coupled Nd ions in ferromagnetically coupled layers perpendicular to the crystal c axis. In contrast, for the $g_y a_x$ ordering of the In compound, the interlayer interaction is antiferromagnetic, the Nd magnetic moments lie in the xy plane and its value is twice larger than in the Ga and Co compounds.

The Nd–Nd superexchange interaction with the each of the six nearest neighbors takes place via four O atoms located approximately at the centers of the edges of the pseudocubic perovskite cell. Our result allows us to conclude that the different Nd–O–Nd angles and distances along the different pathways may affect its strength and character so strongly as to invert its sign and anisotropy.

Table 1
Most relevant refined parameters for $NdCoO_3$ and $NdInO_3$ obtained at $T < T_N$. The standard deviation is in parenthesis. Fractional coordinates have been fixed to their values at RT, as determined by X-ray diffraction [7, 5]

	$NdCoO_3$	$NdInO_3$
T (K)	0.250	0.280
a (Å)	5.353(3)	5.602(3)
b (Å)	5.330(1)	5.875(1)
c (Å)	7.539(3)	8.093(4)
M_x (μ_B)	0	1.21(7)
M_y (μ_B)	0	2.58(8)
M_z (μ_B)	1.39(3)	0
R_{wp} (%)	9.1	7.1

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