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Letter

Magnetic structure of the NaCl-type NdSb compound

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ABSTRACT

Neutron powder diffraction experiments have been carried out on the well-known NaCl-type polycrystalline NdSb compound. The neutron diffraction data obtained in zero field at 2 K, reveal commensurate antiferromagnetic ordering with magnetic moments of Nd directed along *Z* axis (M_{Nd} = 3.1(1) μ_B). Thermal variation of intensity of (0 0 1) magnetic reflection shows the temperature of magnetic ordering at T_N = 13 K.

Well-known NaCl-type NdSb [1] show antiferromagnetic ordering at T_N = 10–16 K with effective magnetic moment $M_{eff}^{Nd} = 3.75\ \mu_B$, paramagnetic temperature $\theta_P = -3$ K [2]. Meantime, the NaCl-type NdAs and NdBi compounds demonstrate the antiferromagnetic commensurate magnetic structure [2].

In order to examine the magnetic structure of NaCl-type NdSb compound, a powder neutron diffraction study was undertaken.

The NdSb compound was prepared by arc melting under argon atmosphere starting from high purity elements (Nd—99.9%, Sb—99.99% pure).

The neutron diffraction investigation was carried out from 90 K down to 2 K in the absence of applied magnetic field the zero at the Institute Laue-Langevin, Grenoble, France, using the high neutron flux powder diffractometer *D1B* [3], operating at a wavelength λ = 0.2524 nm selected by a pyrolitic graphite monochromator. In the configuration used, the resolution of *D1B* was about 0.3° (Full Width at Half Maximum) the multicounter is composed of 400 cells covering a total angular domain of 80° (2θ = 4–84°). The diffraction patterns were indexed, and the calculations performed using the FULLPROF 98-program [4].

The powder neutron diffraction patterns obtained at 90 K and 2 K in zero magnetic field show the development of commensurate reflections (Fig. 1) that correspond to pure antiferromagnetic structure whose details are given in Fig. 2 and Table 1. Thermal variation of intensity of (0 0 1) magnetic reflection shows the temperature of magnetic ordering at T_N = 13 K (Fig. 3a). The

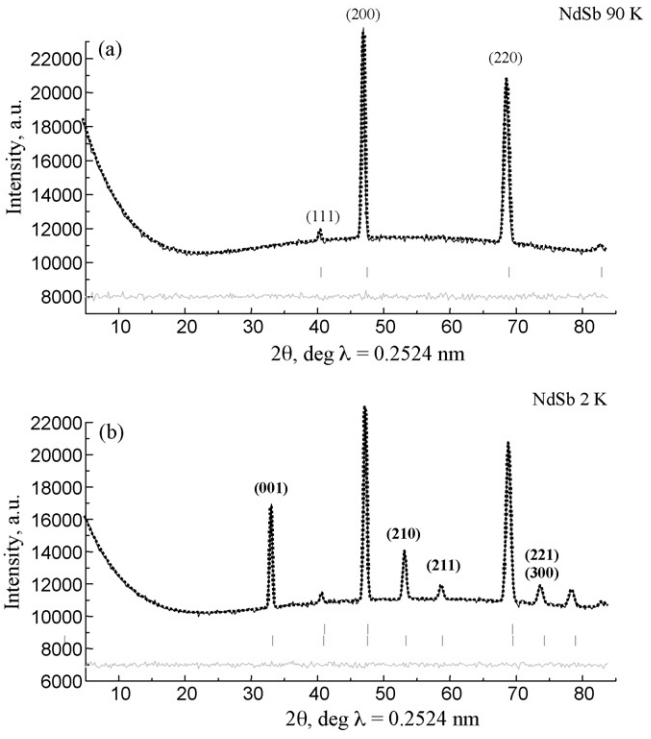

Fig. 1. Neutron diffraction patterns of NdSb at 90 K (paramagnetic state) (a) and at 2 K (commensurate antiferrimagnet) (b).

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Table 1
Crystallographic and magnetic parameters of NaCl-type NdSb compound (space group *Fm*3*m*, No. 225) at different temperatures *T*: magnetic type, unit cell data (cell parameter *a* and atomic position of Nd atoms); temperature T_N refers to a magnetic transition from neutron diffraction experiment; magnetic moment of Nd atom *M*; φ and θ angles (φ the angle of magnetic moment with *X* axis of unit cell and θ the angle of magnetic moment with *Z* axis of unit cell). Reliability factors R_F (crystal structure) and R_F^m (magnetic structure) are given in percent (%).

Magnetic type	T_N (K)	*T* (K)	Unit cell data	R_F (%)	Atom	*M* (μ_B)	φ (°)	θ (°)	R_F^m (%)
Paramagnetic		90	*a* = 0.6338(2) nm	4.4					
Collinear AF	13	2	*a* = 0.6336(2) nm	5.0	Nd1	3.1(1)	0	0	12.0
			Nd1 [0, 0, 0]		Nd2		0	180	
			Nd2 [0, 1/2, 1/2]		Nd3		0	0	
			Nd3 [1/2, 1/2, 0]		Nd4		0	180	
			Nd4 [1/2, 0, 1/2]						

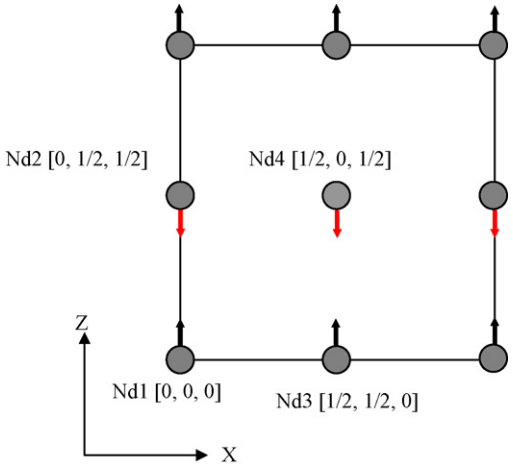

Fig. 2. The magnetic ordering in Cu-type sublattice of NaCl-type NdSb compound.

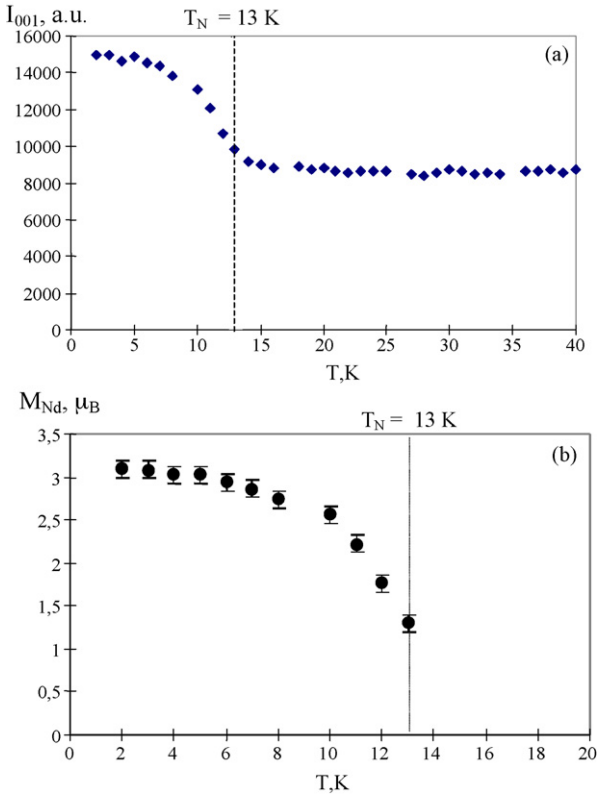

Fig. 3. Thermal variation of intensity I_{001} of magnetic reflection (0 0 1) (a) and magnetic moment of Nd atom (b).

magnitude of Nd magnetic moment rich the 3.1(1) μ_B at 2 K (Fig. 3b).

The magnetic structure of NdSb equals to the magnetic structure of NdAs and NdBi compounds.

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