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Magnetic structure of Nd_7Ni_3

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Abstract

The magnetic structure of a hexagonal intermetallic compound Nd_7Ni_3 has been studied by the neutron diffraction measurements. The Rietveld analysis was carried out to refine the structural and magnetic parameters. The refined propagation vector is $\boldsymbol{Q} = (0\,0\,0.32(2))$ to describe the ferrimagnetic structure at 2.0 K. The magnetic moment of the Nd atom is 2.00(1), 2.09(1), 2.09(1) μ_B for the sites I, II and III, respectively. The magnetic moment at the site I has the conical structure with the cone angle 22.00(1)°. The refined initial relative phase is 39.43(3)° for sites I and II and 41.43(5)° for sites II and III, respectively.

Keywords: Nd_7Ni_3; Neutron diffraction; Magnetic structure; Magnetic moment

1. Introduction

The intermetallic compound Nd_7Ni_3 crystallizes in the Th_7Fe_3 type hexagonal structure with the space group $P6_3mc$ in which the Nd atom occupies three non-equivalent sites [1,2]. From our previous studies, the following results were obtained [3,4]. (1) At 4.2 K, Nd_7Ni_3 possesses ferromagnetic state with small resultant magnetization, 0.15 μ_B/Nd, along the *c*-axis. Two successive metamagnetic transitions take place in the *c*-plane and the saturation magnetization is 2.1 μ_B/Nd. No magnetic anisotropy was observed in the *c*-plane. (2) The spin reorientation takes place at $T_R = 7.8$ K and the easy direction of the resultant magnetization lies in the *c*-plane. In the temperature range from 7.8 K to $T_C = 11.5$ K, Nd_7Ni_3 shows another ferrimagentic state with a small spontaneous magnetization in the *c*-plane and paramagnetic state takes place at $T_N = 25$ K. (3) The neutron diffraction studies have also been carried out at 4.2 K and a commensurate conical magnetic structure has been concluded for the lowest temperature phase with the propagation vector $\boldsymbol{Q} = (0\,0\,1/3)$. An incommensurate distorted helical structure and an incommensurate helical structure have been proposed, respectively, for the second ferrimagentic state in $T_R < T < T_C$ and the antiferromagentic state above T_C [5]. However, any *c*-plane magnetization was not observed for the second ferrimagentic state in the neutron diffraction studies.

In this study, the magnetic structure of Nd_7Ni_3 has been determined for the low temperature ferrimagentic state by the powder neutron diffraction measurement.

2. Experimental

The polycrystalline ingots were prepared by arc-melting the constituent 99.9%-pure Nd and 99.99%-pure Ni elements under high purity argon atmosphere. Powdered samples were annealed at 300 °C for 30 h in an evacuated quartz tube. The powder X-ray diffraction analysis indicated that the samples

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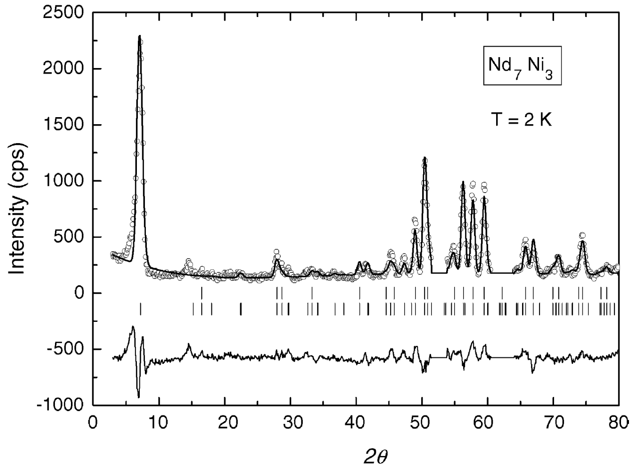

Fig. 1. Neutron diffraction pattern of Nd_7Ni_3 at 2.0 K. Open circles represent the experimental data; the upper vertical bars indicate the Bragg peaks of nuclear and the lower ones indicate the peaks of magnetic origin, respectively. The solid line at the bottom gives the difference between the observed and calculated intensities.

were in single phase with Th_7Fe_3 type hexagonal structure. The neutron diffraction experiments were carried out using the diffractometer HQR installed at JRR-3M of JAERI, Tokai, Japan. The wavelength is 2.448 Å. The Rietveld-type program FullProf was used to refine the crystal and magnetic structure [6].

3. Results and discussion

The diffraction pattern measured at 2.0 K is shown in Fig. 1. The reflections from the cryostat were eliminated in the analysis. The refined structural parameters are listed in Table 1. The R factors, $R_{\mathrm{Bragg}} = 16.1\%$ and $R_{\mathrm{RF}} = 9.37\%$, were obtained. The determined atomic coordinates of the constituent atoms are comparable to those determined by the X-ray and neutron diffractions for Ce_7Ni_3 [2,7].

The magnetic reflections can be indexed by the propagation vector $\boldsymbol{Q} = (0\,0\,1/3)$. Our previous results of magnetization and magnetic susceptibility measurements for Nd_7Ni_3 single crystals indicate that the magnetic moment of Nd tends to lie in the c-plane of the crystal and a small resultant magnetization of 0.15 μ_B/Nd exists along the c-axis [3]. Since the only the site I Nd atom is located at the different crystallographic 6(b) site, we have assumed a conical structure model in which only the Nd atom at the site I has a c-axis component. Table 2 shows the observed and calculated intensity of the magnetic reflections on this model. The propagation vector has been refined to be $\boldsymbol{Q} = (0\,0\,0.32(2))$. The magnetic moment is 2.00(1) μ_B for sites I and II, 2.09(1) μ_B for site III, respectively. The R factor for the magnetic structure refinement was obtained to be $R_m = 10.02\%$. The cone angle θ of the Nd magnetic moment at the site I is 22.00(1)° and that for the sites II and the site III is 0.0(0)°.

Fig. 2 shows a possible magnetic structure of Nd_7Ni_3 at 2.0 K. In this figure the initial phase of site II is zero at $z = 0.01$. The magnetic moment of Nd is described by both the c-axis and c-plane components $\mu_v = \mu_0 \sin\theta$ and $\mu_h = \mu_0 \cos\theta$ for each site, where μ_0 is the magnetic moment of the Nd atom. The magnetic moment parallel and perpendicular to the c-axis for the three different sites can be expressed as follows,

$$\mu_{1xy} = \mu_{1h} \sin(Q_z z + \phi_1)$$
$$\mu_{1z} = \mu_v \tag{1}$$

Table 1
Refined structural parameters of Nd_7Ni_3 at 2.0 K

$P6_3mc$ (no. 186)		$a = 9.8732$ Å, $c = 6.2977$ Å		
Atom	Site	x	y	z
Nd1	2(b)	0.3211	0.6449	0.8008
Nd2	6(c)	0.1229	0.8818	0.0108
Nd3	6(c)	0.5327	0.4539	0.8226
Ni	6(c)	0.8099	0.1823	0.0748

Table 2
Observed and calculated integrated intensity of magnetic reflections at 2.0 K

h	k	l	F^2 (observed)	F^2 (calculated)
0	0	0.3212	53.016	51.757
0	1	0.3212	0.149	0.106
0	2	0.3212	1.315	1.888
0	4	0.3212	0.716	0.94
0	2	1.3212	5.979	4.156
0	1	1.6788	5.917	8.984
0	2	1.6788	3.679	7.988
0	1	2.3212	5.791	6.07
0	1	2.6788	0.533	0.373
0	2	2.6788	3.612	5.716
1	0	0.3212	0.253	0.18
1	1	0.3212	2.159	0.343
1	2	0.3212	3.686	2.674
1	0	0.6788	1.439	1.33
1	1	0.6788	0.823	0.067
1	1	1.3212	0.034	0.067
1	2	1.3212	6.024	5.125
1	2	1.6788	0.359	0.354
1	2	2.3212	0.287	0.325
1	0	2.6788	0.446	0.313
1	1	2.6788	0.094	0.12
2	0	0.3212	1.346	1.932
2	2	0.3212	3.061	2.989
2	1	0.6788	7.186	5.091
2	1	1.3212	8.697	7.398
2	0	1.6788	3.21	6.97
2	1	2.3212	0.843	0.954
3	2	0.3212	0.818	0.836
3	0	1.6788	0.564	0.39
3	1	1.6788	0.011	0.445
3	0	2.3212	2.219	4.367
4	0	0.3212	0.22	0.289
4	0	0.6788	0.711	1.388

$\boldsymbol{Q} = (0\,0\,0.32(2))$.

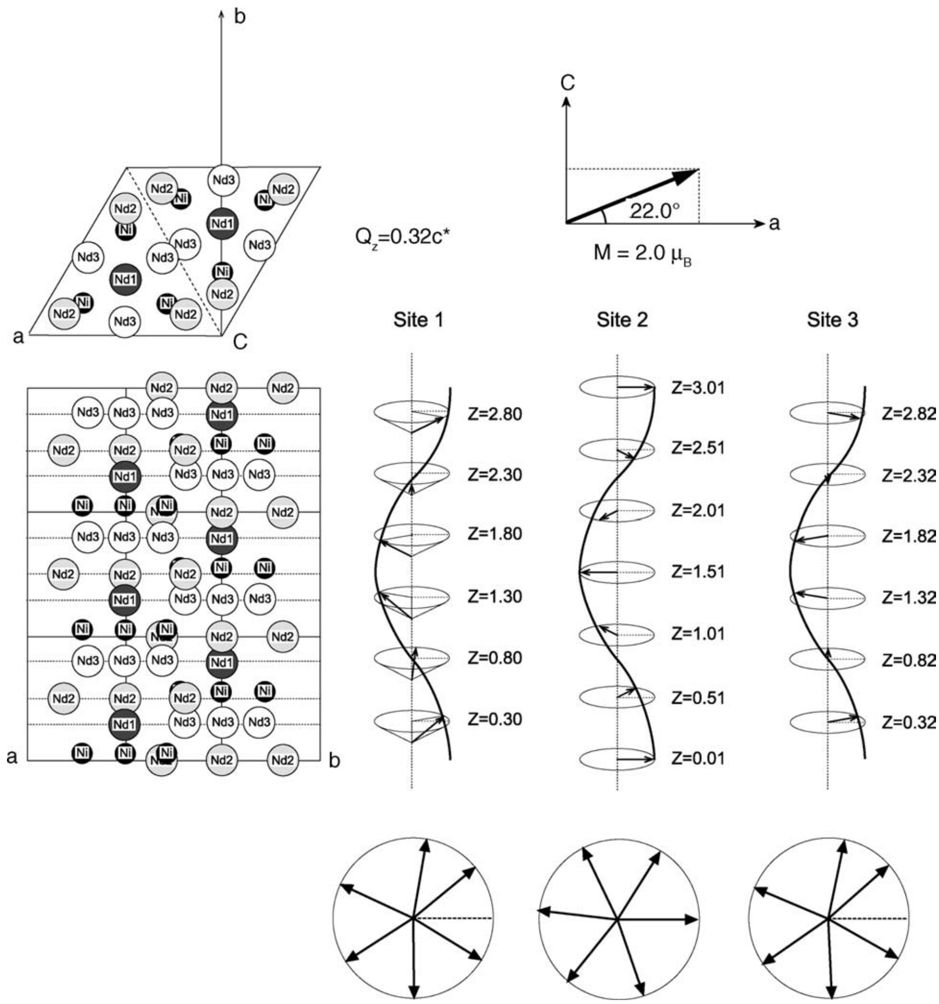

Fig. 2. The magnetic structure of Nd_7Ni_3 at 2.0 K.

for the site I and

$$\begin{aligned} \mu_{2xy} &= \mu_{2h}\ \sin(Q_z z + \phi_2) \\ \mu_{3xy} &= \mu_{3h}\ \sin(Q_z z + \phi_3) \\ \mu_{2z} &= \mu_{3z} = 0 \end{aligned} \tag{2}$$

for the sites II and III, respectively. Here, $\boldsymbol{Q}_z$ is the propagation vector component along the c-axis, ϕ_1, ϕ_2 and ϕ_3 are the initial phase for each site. The refined initial relative phase is 39.43(3)° for sites I and II, 41.43(5)° for sites II and III, respectively. From these results, the magnetization along the c-axis is evaluated to be $M_z = 0.11\ \mu_B$/Nd. This value is in a reasonable agreement with the bulk magnetization measurement results of $M_z = 0.15\ \mu_B$/Nd at 4.2 K [3].

For further investigations, neutron diffraction studies for the magnetic structure in the hith temperature ferrimagnetic phase and the antiferromagentic phase are now in progress.

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