Neutron Diffraction Studies of $NdNi_5Sn$ Compound

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The neutron powder diffraction measurements of the $NdNi_5Sn$ compound have been performed. The obtained results indicate that this compound crystallizes in a hexagonal $CeNi_5Sn$-type crystal structure described by the space group $P6_3/mmc$. The parameters of the crystal structure at 1.55 and 14.8 K are determined. In contradiction to the magnetic data the long-range magnetic ordering was not detected up to 1.55 K.

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1. Introduction

The magnetic properties of RNi_5Sn compounds are the object of our investigations. These compounds for R = La–Nd crystallize in a hexagonal crystal structure (space group $P6_3/mmc$) with a complex crystal structure [1]. Preliminary magnetic measurements performed in the temperature range 80–400 K indicate paramagnetic properties [2]. New ac and dc magnetic data indicate for $NdNi_5Sn$ below the Néel temperature equal to 8.8 K — the complex magnetic properties [3]. Presented in Ref. [3] data suggest the neutron diffraction experiment for determining the magnetic structure of this compound. This work reports the results of these investigations at low temperatures.

2. Experimental data and results

The experiment is performed on the sample which preparation and X-ray analysis is descripted in Ref. [3]. The neutron diffractograms were obtained at temperature equal to 1.55 and 14.8 K with use of the E6 diffractometer at BERII reactor (Helmholtz-Zentrum Berlin). The incident neutron wavelength was 2.447 Å. The data were analyzed using the Rietveld-type program FullProf [4].

The neutron diffraction pattern measured at 1.55 K is shown in Fig. 1. Similar neutron pattern is observed at 14.8 K. Analysis of these data confirm that the investigated compound crystallizes in a hexagonal crystal structure (space group $P6_3/mmc$) with the following distribution of atoms: Nd_1 in $2c$ site: 1/3, 2/3, 1/4; Nd_2 in $2a$ site: 0, 0, 0; Ni atoms occupy four sublattices: Ni_1 in $2b$ site: 0, 0, 1/4; Ni_2 in $2d$ site: 1/3, 2/3, 3/4; Ni_3 in $4f$ site: 1/3, 2/3, z_1; Ni_4 in $12k$ site: x, y, z_2 and Sn atoms in $4f$ site: 1/3, 2/3, z_3. The determined crystal structure parameters are collected in Table. These parameters agree well with the published previously data [1, 3]. Comparison of the data from 1.55 K with those from 14.8 K does not give evidence for the additional peaks connected with magnetic origin (see lower part in Fig. 1). This result suggests the absence of the long range magnetic order and is in contradiction with the previous magnetic data [3]. These data in temperature dependence of the χ' and χ'' components of ac magnetic susceptibility give the anomalies at 8.8 K (see Fig. 3 in Ref. [3]) and the small ferromagnetic component with the small hysteresis in the magnetization curve (see inset in Fig. 2b in Ref. [3]).

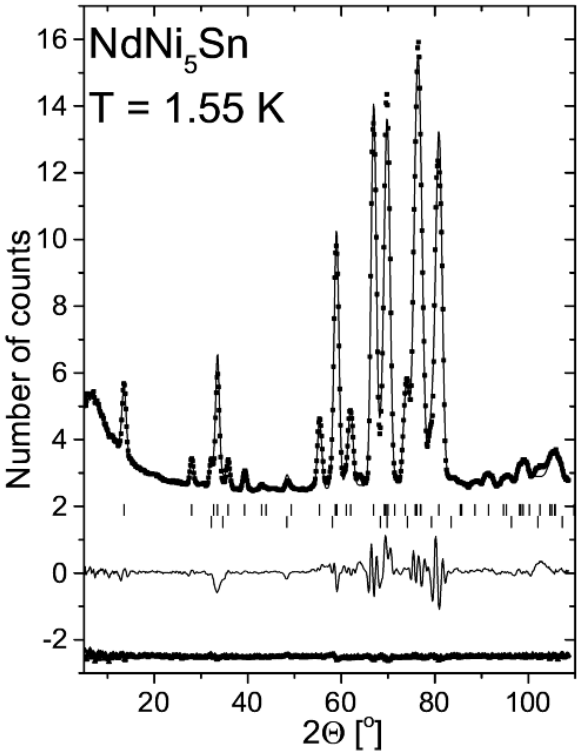

Fig. 1. Comparison between the observed and calculated neutron diffraction pattern by the Rietveld method at 1.55 K. The symbols represent the experimental data while the solid line denotes the calculated profile. The difference between the observed and calculated intensities is shown at the bottom of diagram. The vertical bars indicate the positions of the Bragg peaks for $NdNi_5Sn$ (first row) and $NdNi_5$ (second row). In the lower part the difference between patterns collected in 1.55 and 14.8 K is presented.

TABLE

Crystal and structure parameters of $NdNi_5Sn$ compounds determined from the neutron diffraction data at 1.55 and 14.8 K.

Parameter	$T = 1.55$ K	$T = 14.8$ K
a [Å]	4.9111(11)	4.9111(12)
c [Å]	19.7524(53)	19.7525(55)
V [Å^3]	412.58(28)	412.58(30)
Ni_3 z_1	0.5430(3)	0.5430(3)
Ni_4 x	0.8310(3)	0.8310(3)
y	0.6625(3)	0.6625(2)
z_2	0.1459(2)	0.1460(2)
Sn z_3	0.0865(5)	0.0864(6)
R_{Bragg} [%]	4.92	5.07
R_{F} [%]	3.44	3.62

Observed anomalies are probably connected with the impurity phase $NdNi_5$. This compound is ferromagnet with the Curie temperature 7 K [5]. The existence of this phase is not observed in the X-ray experiment while in the neutron diffraction patterns the small intensity peak at $2\theta = 48.5^\circ$ indicate nearly 4% impurity phase $NdNi_5$ which crystallizes in a hexagonal $CaCu_5$-type crystal structure (space group $P6/mmm$) with the Nd atoms in $1a$ site: 0, 0, 0 and Ni atoms in $2c$: 1/3, 2/3, 0 and $3g$: 1/2, 0, 1/2 sites. Numerical analysis of our data confirm this structure with the lattice parameters $a = 4.9866(23)$ Å and $c = 4.0259(17)$ Å and $R_{\mathrm{Bragg}} = 10.4\%$ and $R_{\mathrm{F}} = 6.7\%$.

Crystal chemical analysis [6] shown that the crystal structure of the $NdNi_5Sn$ compound can be considered as consisting of two kinds of layers, with stoichiometry $NdNi_5$ and $NdNi_5Sn_2$, which stack alternately along [001] of the hexagonal unit cell (see Fig. 2 in Ref. [6]) with the sequence 1:1. In $NdNi_5Sn$ compound the Nd and Ni atoms form a close packing site. During thermal treatment in the part of sample the impurity phase $NdNi_5$ is pushed out.

Presented results confirm that up to 1.55 K the long range order does not exist.

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