

Neutron Diffraction Studies of NdNi₅Sn Compound

B. PENC^a, S. BARAN^a, A. HOSER^b, L.P. ROMAŁA^c AND A. SZYTUŁA^a

^aM. Smoluchowski Institute of Physics, Jagiellonian University, W.S. Reymonta 4, 30-059 Kraków, Poland

^bHelmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Pl. 1, D-14 109 Berlin, Germany

^cDepartment of Inorganic Chemistry, Lviv National University, Kyryla and Mephodiy 6, 79005 Lviv, Ukraine

The neutron powder diffraction measurements of the NdNi₅Sn compound have been performed. The obtained results indicate that this compound crystallizes in a hexagonal CeNi₅Sn-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 RNi₅Sn 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 NdNi₅Sn 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 described 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: Nd₁ in 2c site: 1/3, 2/3, 1/4; Nd₂ in 2a site: 0, 0, 0; Ni atoms occupy four sublattices: Ni₁ in 2b site: 0, 0, 1/4; Ni₂ in 2d site: 1/3, 2/3, 3/4; Ni₃ in 4f site: 1/3, 2/3, z₁; Ni₄ in 12k site: x, y, z₂ and Sn atoms in 4f site: 1/3, 2/3, z₃. 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

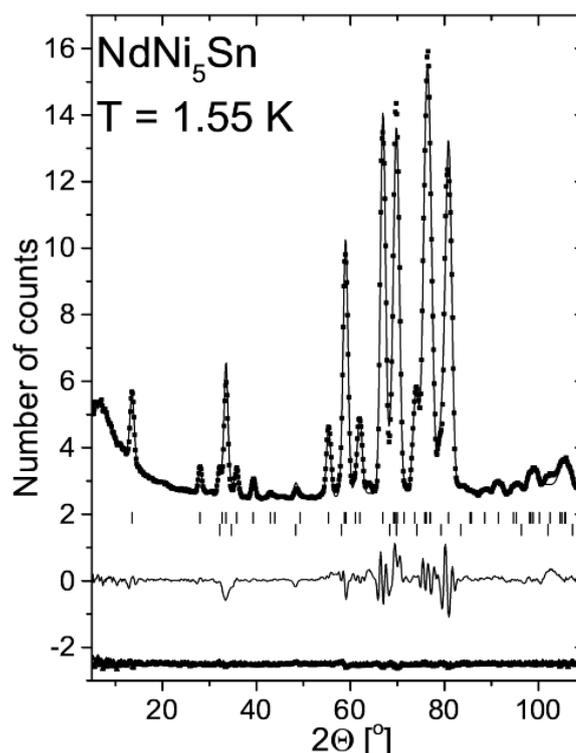


Fig. 1. Comparison between the observed and calculated neutron diffraction pattern by the Rietveld method at 1.55 K. The symbols represent the experimental data while the solid line denotes the calculated profile. The difference between the observed and calculated intensities is shown at the bottom of diagram. The vertical bars indicate the positions of the Bragg peaks for NdNi₅Sn (first row) and NdNi₅ (second row). In the lower part the difference between patterns collected in 1.55 and 14.8 K is presented.

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]).

TABLE

Crystal and structure parameters of NdNi₅Sn 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 NdNi₅. 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 NdNi₅ which crystallizes in a hexagonal CaCu₅-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 $R_{\text{Bragg}} = 10.4\%$ and $R_{\text{F}} = 6.7\%$.

Crystal chemical analysis [6] shown that the crystal structure of the NdNi₅Sn compound can be considered as consisting of two kinds of layers, with stoichiometry NdNi₅ and NdNi₅Sn₂, which stack alternately along [001] of the hexagonal unit cell (see Fig. 2 in Ref. [6]) with the sequence 1:1. In NdNi₅Sn compound the Nd and Ni atoms form a close packing site. During thermal treatment in the part of sample the impurity phase NdNi₅ is pushed out.

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

Acknowledgments

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