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Single-crystal structure investigation of NdNi and $NdNi_5$

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Abstract

The structures of NdNi and $NdNi_5$ have been determined by single-crystal data. NdNi crystallizes in the orthorhombic space group *Cmcm* (No. 63), with $a=3.8059(5)$ Å, $b=10.462(4)$ Å, $c=4.3345(12)$ Å, $Z=4$, $V=172.59(8)$ Å^3 and the BCr structure type. $NdNi_5$ crystallizes with the $CaCu_5$ structure type, space group *P6/mmm* (No. 191), $a=4.973(2)$ Å, $c=4.0124(11)$ Å, $Z=1$ and $V=85.94(5)$ Å^3.

Keywords: Rare earth compounds; Transition metal compound; X-ray diffraction; Structure determination

1. Introduction

The crystallographic data available for the compounds RNi and RNi_5 (R=La, Ce, Pr, Nd, Tb, Sm, Eu) are from X-ray powder methods only [1]. This paper is part of a systematic structural study of the compounds in the R–T–Ge systems (T represents Ni or Fe). We therefore report the structures of NdNi and $NdNi_5$ as refined by single-crystal methods.

2. Experimental and results

Cylinder-like single crystals of NdNi and $NdNi_5$ were obtained during the preparation of the ternary alloys $Nd_{50}Ni_{44}Ge_6$ and $Nd_{18}Ni_{77}Ge_5$, respectively, which were prepared by arc melting and annealing at 1023 K for 600 h. Starting materials were neodymium foil (Ames Lab. 99.6%), powders of nickel (Fisher, purified powder) and germanium (Alfa, −100 mesh, 99.999%). Before melting, stoichiometric quantities of nickel and germanium powder were mixed and cold-pressed.

Cylinder-like single crystals were selected and measured using Rigaku AFC6R diffractometer and the crystallographic data for NdNi and $NdNi_5$ are listed in Table 1. The final structural data for the compounds are given in Tables 2 and 3. NdNi crystallizes with the BCr structure type [2]. Its structural projection is shown in Fig. 1. The structure contains two different coordination polyhedra: Nd $[Nd_6Ni_7]$ and Ni $[Nd_7Ni_2]$. $NdNi_5$ crystallizes with the $CaCu_5$ structure type [3]. Fig. 2 shows its projection along [001]. The structure contains the following coordination polyhedra: Nd $[Ni_{18}]$, Ni $[Nd_3Ni_6]$ and Ni $[Nd_4Ni_8]$.

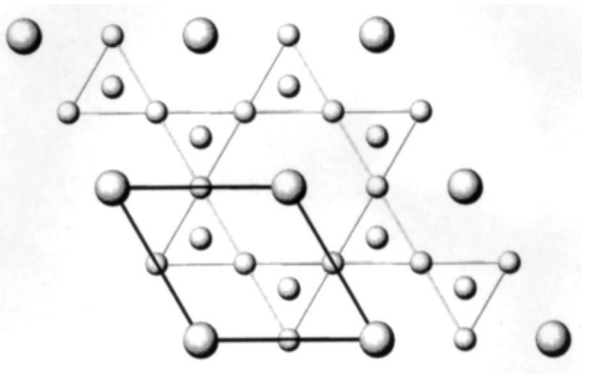

Fig. 1. Structural projection of NdNi along [100]; large circles, Nd; small circles, Ni.

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Table 1
Crystallographic data for NdNi and $NdNi_5$

Formula	NdNi	$NdNi_5$
Formula mass	202.95	437.79
Space group	*Cmcm*	*P6/mmm*
a (Å)	3.8059(5)	4.973(2)
b (Å)	10.462(4)	4.973(2)
c (Å)	4.3345(12)	4.0124(11)
V ($Å^3$)	172.59(8)	85.94(5)
Z	4	1
T (K)	293(2)	293(2)
D ($\times g\ cm^{-3}$)	7.811	8.459
Diffractometer	Rigaku AFC6R	Rigaku AFC6R
Crystal dimensions (mm)	0.12×0.05×0.036	0.14×0.06×0.045
Radiation (monochromated In incident beam)	Mo Kα (0.71069 Å)	Mo Kα (0.71069 Å)
Absorption factors	402.400	415.365
Data collected	$0\leqslant h\leqslant 4$, $0\leqslant k\leqslant 12$, $0\leqslant l\leqslant 5$	$0\leqslant h\leqslant 6$, $0\leqslant k\leqslant 4$, $0\leqslant l\leqslant 6$
No. of reflections	94	80
No. of refined parameter	9	8
R	0.008	0.032
w*R*	0.011	0.028
Goodness of fit	1.533	2.455
Structure solution program	TEXSAN [4]	TEXSAN

Table 2
Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for NdNi and $NdNi_5$

Atom	Wyckoff position	*x*	*y*	*z*	Occ.	B_{eq}
NdNi						
Nd	4*c*	0	0.13851(5)	1/4	1	1.099(2)
Ni	4*c*	0	0.4273(1)	1/4	1	1.384(5)
$NdNi_5$						
Nd	1*a*	0	0	0	1	0.91(4)
Ni(1)	2*c*	1/3	2/3	0	1	0.63(5)
Ni(2)	3*g*	1/2	0	1/2	1	0.70(1)

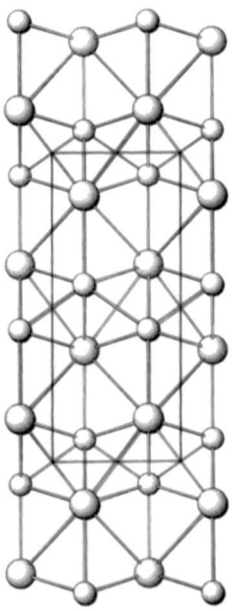

Fig. 2. Structural projection of $NdNi_5$ along [001]; large circles, Nd; small circles, Ni.

Table 3
Selected interatomic distances (Å) for NdNi and $NdNi_5$

NdNi			
Nd–Nd	3.619(1)	Nd–Nd	3.7096(9)
Nd–Ni	3.021(2)	Nd–Ni	2.9650(6)
Nd–Ni	2.916(1)	Ni–Ni	2.648(2)
$NdNi_5$			
Nd–Ni(1)	2.8713(12)	Nd–Ni(1)	2.8709(7)
Nd–Ni(2)	3.1950(8)	Ni(1)–Ni(1)	2.8713(12)
Ni(1)–Ni(2)	2.4670(6)	Ni(2)–Ni(2)	2.4866(10)

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