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COMMUNICATION

Crystal Structure of Nd_2Ni_2Pb and Nd_5NiPb_3 Compounds

by L.D. Gulay[*] and M. Wołcyrz[**]

W. Trzebiatowski Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 1410, 50-950 Wrocław, Poland

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The only crystal structures of Nd–Ni–Pb ternaries studied so far were $Nd_{12}Ni_6Pb$ ($Sm_{12}Ni_6In$-type structure, space group *Im3*, $a = 9.932$ Å) [1] and NdNiPb (TiNiSi-type structure, space group *Pnma*, $a = 7.4249$ Å, $b = 4.6116$ Å, $c = 7.8238$ Å) [2]. The present paper reports the results of the crystal structure investigation of two new phases: Nd_2Ni_2Pb and Nd_5NiPb_3. The samples with a total mass of about 1 g were prepared by arc melting of pure metals (the purity of ingredients was better than 99.9 wt. %) in a high-purity argon atmosphere. All alloys were remelted twice to ensure homogeneity. The mass losses after the melting were less than 1 wt. %. After melting the samples were sealed in evacuated quartz ampoules and annealed at 870 K during 720 h. Then the ampoules were quenched in cold water. Two new compounds with the nominal compositions of $Nd_{40}Ni_{40}Pb_{20}$ and $Nd_{56}Ni_{11}Pb_{33}$ were found.

X-ray powder diffraction diagrams for phase analysis were recorded using a DRON-2.0 powder diffractometer (FeK_α radiation, $20° \leq 2\Theta \leq 100°$, silicon powder as an internal standard). The diffraction data for crystal structure determination were collected using a Siemens D5000 powder diffractometer (CuK_α radiation, $10° \leq 2\Theta \leq 120°$, step scan mode with a step size of 0.02° and counting time of 15 s per data point). The lattice parameters were calculated by least-squares method. Crystal structure refinements were performed by the Rietveld method using the DBWS-9411 program [3].

The X-ray powder diffraction diagram of the $Nd_{40}Ni_{40}Pb_{20}$ sample was indexed in the orthorhombic unit cell with the lattice parameters listed in Table 1. The composition of the sample, intensities of the reflections and lattice parameters proved that the compound is isostructural with the Mn_2AlB_2 (space group *Cmmm*) [4]. The results of the crystal structure determination are given in Table 1. Atomic and thermal parameters are listed in Table 2.

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[*] On leave from the Inorganic Chemistry Department, Lviv National University, Lviv, Ukraine.
[**] To whom all correspondence should be addressed.

The X-ray powder diffraction diagram of the $Nd_{56}Ni_{11}Pb_{33}$ sample was indexed assuming a hexagonal unit cell with the lattice parameters listed in Table 1. Hf_5CuSn_3-type structure (space group *P6₃/mcm*) [5,6] was chosen as the model for the crystal structure refinement. The results are collected in Tables 1 and 2. Interatomic distances for the Nd_2Ni_2Pb and Nd_5NiPb_3 compounds are listed in Table 3. They agree with the sum of atomic radii of the respective atoms.

Table 1. Results of the crystal structure determination of the Nd_2Ni_2Pb and Nd_5NiPb_3 compounds.

Compound	Nd_2Ni_2Pb	Nd_5NiPb_3
Structure type	Mn_2AlB_2	Hf_5CuSn_3
Space group	*Cmmm*	*P6₃/mcm*
a (Å)	4.1344(7)	9.280(1)
b (Å)	14.283(1)	9.280(1)
c (Å)	3.7459(6)	6.7767(5)
V (Å^3)	221.20(9)	505.4(1)
Z	2	2
Calculated density (g/cm^3)	9.204	9.208
Cu K_α wavelength (Å)	1.54178	1.54178
Mode of refinement	full profile	full profile
R_P	0.045	0.054
R_{wP}	0.068	0.070

Table 2. Atomic and thermal parameters of Nd_2Ni_2Pb and Nd_5NiPb_3 compounds.

Nd_2Ni_2Pb					
atom	Wyckoff position	*x*	*y*	*z*	B (Å^2)
Nd	4(*j*)	0	0.3610(1)	1/2	1.1(1)
Ni	4(*i*)	0	0.2063(4)	0	1.6(3)
Pb	2(*a*)	0	0	0	0.9(1)
Nd_5NiPb_3					
atom	Wyckoff position	*x*	*y*	*z*	B (Å^2)
Nd1	6(*g*)	0.2226(6)	0	1/4	1.0(1)
Nd2	4(*d*)	1/3	2/3	0	0.5(1)
Ni	2(*b*)	0	0	0	1.8(3)
Pb	6(*g*)	0.5987(4)	0	1/4	0.3(1)

Table 3. Interatomic distances for the Nd_2Ni_2Pb and Nd_5NiPb_3 compounds.

		Nd_2Ni_2Pb		
Nd	2 Ni 2.897(5)	4 Pb 3.424(1)	2 Nd 3.785(2)	2 Nd 4.1344(7)
	4 Ni 2.950(2)	2 Nd 3.7459(6)	1 Nd 3.971(2)	
Ni	2 Ni 2.415(4)	2 Nd 2.897(5)	1 Pb 2.947(6)	4 Nd 2.950(2)
Pb	2 Ni 2.947(6)	8 Nd 3.424(1)	2 Pb 3.7459(6)	2 Pb 4.1344(7)
		Nd_5NiPb_3		
Nd1	2 Ni 2.672(4)	1 Pb 3.490(7)	2 Pb 3.772(3)	4 Nd2 4.083(4)
	2 Pb 3.232(2)	2 Nd1 3.578(7)	4 Nd1 3.968(3)	
Nd2	6 Pb 3.299(1)	2 Nd2 3.3884(5)	6 Nd1 4.083(4)	
Ni	6 Nd1 2.672(4)			
Pb	2 Nd1 3.232(5)	1 Nd1 3.490(7)	2 Pb 3.852(3)	
	4 Nd2 3.299(1)	2 Nd1 3.772(3)		

The result presented here fill a gap in our knowledge on the constitution of the R_2Ni_2Pb phases. Now, also neodymium representative can be added to the series of the known R_2Ni_2Pb compounds (R = Y, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu) [7]. All these phases have the same, Mn_2AlB_2-type structure.

In comparison with Nd_5NiPb_3, which, as we stated here, crystallizes with the Hf_5CuSn_3-type structure, its lanthanum equivalent, La_5NiPb_3, crystallizes with the Ti_5Ga_4 -type structure [8] which is a disordered variant of Hf_5CuSn_3.

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