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Journal of Alloys and Compounds 311 (2000) 238–240

Journal of ALLOYS AND COMPOUNDS

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Crystal structure of $R_{12}Ni_6Pb$ (R=Y, La, Pr, Nd, Sm, Gd, Tb, Dy, Ho) and $R_{12}Co_6Pb$ (R=Y, La, Pr, Nd, Sm, Gd) compounds

L.D. Gulay[a,*,1], Ya.M. Kalychak[b], M. Wołcyrz[a], K. Łukaszewicz[a]

[a]*W. Trzebiatowski Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna Street 2, P.O. Box 1410, 50-950 Wrocław, Poland*

[b]*Department of Inorganic Chemistry, L'viv Ivan Franko National University, Kyryla and Mefodia Street 6, 79005 L'viv, Ukraine*

Received 31 May 2000; accepted 28 June 2000

Abstract

The crystal structures of the $R_{12}Ni_6Pb$ (R=Y, La, Pr, Nd, Sm, Gd, Tb, Dy, Ho) and the $R_{12}Co_6Pb$ (R=Y, La, Pr, Nd, Sm, Gd) compounds were investigated by powder X-ray diffraction method. They crystallize with $Sm_{12}Ni_6In$ structure type (space group *Im3*, Pearson code *cI38*).

Keywords: Ternary intermetallic compounds; Arc melting; X-ray diffraction; Crystal structure

1. Introduction

Rare earth–nickel (cobalt)–lead ternary systems have not been studied systematicaly until now. Only the crystal structures of the La_5MPb_3 (M=Co, Ni) compounds with Ti_5Ga_4 structure type (space group $P6_3/mcm$) [1] and the $La_6Co_{13}Pb$ compound with $La_6Co_{11}Ga_3$ structure type (space group *I4/mcm*) [2] have been determined. We have found new ternary $R_{12}M_6Pb$ (R=Y, La, Pr, Nd, Sm, Gd, Tb, Dy, Ho; M=Ni and R=Y, La, Pr, Nd, Sm, Gd; M=Co) compounds during the investigation of the phase diagrams of the R–Co(Ni)–Pb ternary systems. Our results of the crystal structure determination of these new compounds are presented in this paper.

2. Experimental details

The samples, each with a total mass of 1 g, were prepared by arc-meltig of pure components (the purity of ingradients was better than 99.9 wt.%) under high-purity argon atmosphere. The ingots were remelted twice to ensure homogeneity. The weight losses after the melting were less than 1%. Homogenizing annealing was carried out at 670 K (or 870 K) for 720 h in evacuated quartz tubes. After the thermal treatment the ampules with samples were quenched in cold water.

The crystal structures of the compounds were determined using powder X-ray diffraction. Powder diffractograms of all samples were obtained using a DRON-2.0 powder diffractometer (FeKα radiation, $20.00 \leq 2\Theta \leq 100.00$, Si as internal standard). These data were used for phase analysis and lattice parameters determination. Intensity data collection for crystal structure determination of the sample with $Y_{63}Ni_{32}Pb_5$ composition was performed using a Siemens D5000 automatic powder diffractometer (CuKα radiation, $10.00 \leq 2\Theta \leq 120.00$, step-scan mode with a step size of 0.02° and counting time of 19 s per data point).

Lattice parameters were calculated using a least squares method. The crystal structure determination was performed using the program DBWS-9411 [4].

3. Results and discussion

The X-ray reflections of the $Y_{63}Ni_{32}Pb_5$ sample were indexed in a cubic cell (a=9.7149(2) Å). The composition of the sample, intensities of reflections and calculated lattice parameters proved that this compound is isostructur-

*Corresponding author.

E-mail address: damm@highscreen.int.pan.wroc.pl (L.D. Gulay).

[1]On leave from the Inorganic Chemistry Department, L'viv National University, L'viv, Ukraine.

0925-8388/00/$ – see front matter
PII: S0925-8388(00)01115-4

Table 1
Crystal data and refinement results for the $Y_{12}Ni_6Pb$ compound

Formula	$Y_{12}Ni_6Pb$
Number of formula units per unit cell	$Z=2$
Structure type	$Sm_{12}Ni_6In$
Space group	*Im3*
a (Å)	9.7149(2)
V (Å^3)	916.89(6)
Calculated density (g/cm^3)	5.890
Radiation and wavelenght (Å)	Cu 1.54178
Diffractometer	Siemens D5000
Mode of refinement	Full profile
R_P	0.0277
R_{wP}	0.0396

Table 2
Atomic and thermal parameters for the $Y_{12}Ni_6Pb$ compound

Atom	Position	x/a	y/b	z/c	$B_{eq.}$ (Å^2)
Y	24(g)	0	0.1888(2)	0.6986(2)	1.22(6)
Ni	12(e)	0.1200(4)	0	1/2	1.71(9)
Pb	2(a)	0	0	0	0.86(4)

al with the $Sm_{12}Ni_6In$ (space group *Im3*, $a=9.800$ Å) compound [3]. Crystal data and refinement results for the $Y_{12}Ni_6Pb$ compound are given in Table 1, whereas atomic and thermal parameters are given in Table 2. The projection of the crystal structure of the $Y_{12}Ni_6Pb$ compound on the *XY* plane and the coordination polyhedra of the Y (a), Ni (b) and Pb (c) atoms are shown in Fig. 1. The Sm atoms form 15-vertices (c.n.=15), the Ni atoms form trigonal prisms with three additional atoms capted four-corners faces (c.n.=9) and the Pb atoms form icosahedrons (c.n.=12). Interatomic distances (δ), Δ values ($\Delta=100(\delta-\Sigma_r)/\Sigma_r$, Σ_r is the sum of the respective atomic radii) and coordination numbers of the atoms are given in Table 3 (the values of atomic radii are taken from Ref. [5]). Some Y–Ni and Ni–Ni distances are significantly shorter than the sum of the respective atomic radii. It means that there exists strong interactions between some Y–Ni and Ni–Ni atoms.

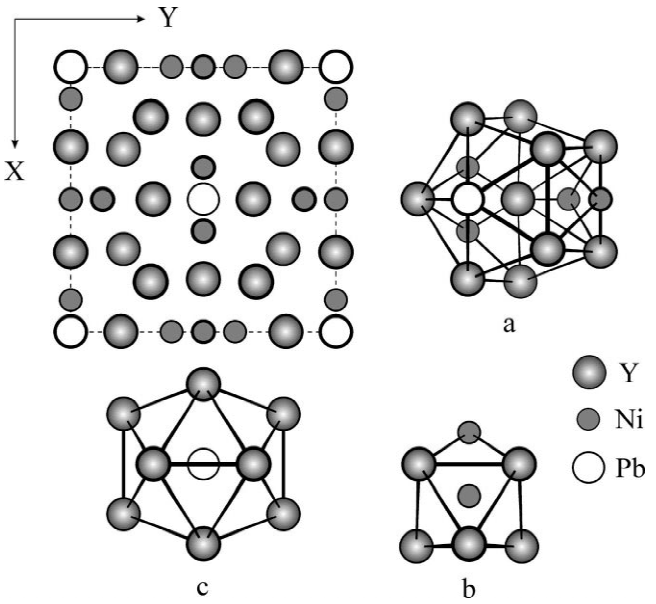

Fig. 1. Projection of the crystal structure of $Y_{12}Ni_6Pb$ on the *XY* plane and coordination polyhedra of the Y (a), Ni (b) and Pb (c) atoms.

Table 3
Interatomic distances (δ, Å), Δ values ($\Delta=100(\delta-\Sigma_r)/\Sigma_r$, Σ_r is the sum of the respective atomic radii) and coordination numbers (c.n.) of the atoms in the $Y_{12}Ni_6Pb$ compound

Atoms		δ (Å)	$\Delta=100(\delta-\Sigma_r)/\Sigma_r$	c.n.
Y–	1Ni	2.678(3)	−12.20	
	2Ni	2.906(2)	−4.72	
	1Pb	3.455(2)	−2.95	
	1Ni	3.499(3)	+14.72	15
	4Y	3.588(2)	−0.88	
	4Y	3.624(2)	+0.11	
	1Y	3.668(3)	+1.32	
	1Y	3.859(3)	+6.60	
Ni–	1Ni	2.332(6)	−5.97	
	2Y	2.678(3)	−12.20	9
	4Y	2.906(2)	−4.72	
	2Y	3.499(3)	+14.72	
Pb–	12Y	3.455(2)	−2.95	12

The $R_{12}Ni_6Pb$ (R=La, Pr, Nd, Sm, Gd, Tb, Dy, Ho) and $R_{12}Co_6Pb$ (R=Y, La, Pr, Nd, Sm, Gd) compounds are isostructural with $Y_{12}Ni_6Pb$. Unit cell parameters, calculated density and annealing temperature for all these compounds are given in Table 4. Unit cell volumes of these compounds are shown in Fig. 2. The data are in good

Table 4
Unit cell parameters, calculated density and annealed temperature for $R_{12}Ni_6Pb$ (R=Y, La, Pr, Nd, Sm, Gd, Tb, Dy, Ho) and $R_{12}Co_6Pb$ (R=Y, La, Pr, Nd, Sm, Gd) compounds

Compound	a (Å)	V (Å^3)	Calculated density	Annealed temperature (K)
$Y_{12}Ni_6Pb$	9.7149(2)	916.89(6)	5.890	870
$La_{12}Ni_6Pb$	10.233(2)	1071.5(6)	6.900	670
$Pr_{12}Ni_6Pb$	9.954(1)	986.3(3)	7.577	670
$Nd_{12}Ni_6Pb$	9.932(2)	979.7(6)	7.763	670
$Sm_{12}Ni_6Pb$	9.825(2)	948.4(6)	8.276	670
$Gd_{12}Ni_6Pb$	9.770(2)	932.6(6)	8.712	870
$Tb_{12}Ni_6Pb$	9.707(2)	914.7(6)	8.955	870
$Dy_{12}Ni_6Pb$	9.662(1)	902.0(3)	9.239	870
$Ho_{12}Ni_6Pb$	9.604(2)	885.8(6)	9.517	870
$Y_{12}Co_6Pb$	9.686(1)	908.7(3)	5.948	870
$La_{12}Co_6Pb$	10.161(2)	1049.1(6)	7.052	670
$Pr_{12}Co_6Pb$	9.930(2)	979.1(6)	7.637	670
$Nd_{12}Co_6Pb$	9.877(2)	963.6(6)	7.898	670
$Sm_{12}Co_6Pb$	9.780(1)	935.4(3)	8.396	670
$Gd_{12}Co_6Pb$	9.727(2)	920.3(6)	8.832	870

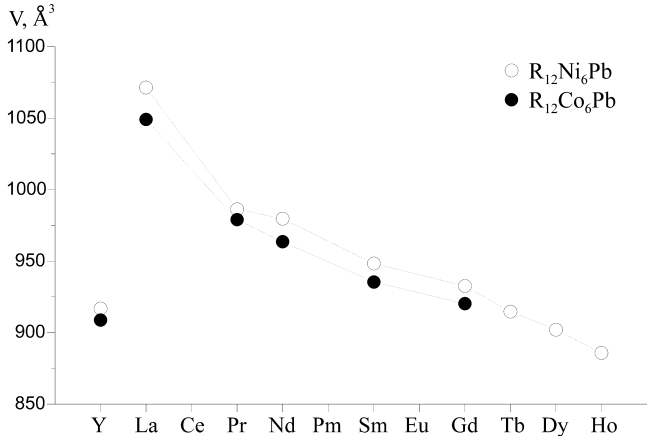

Fig. 2. Unit cell volume of $R_{12}Ni_6Pb$ (R=Y, La, Pr, Nd, Sm, Gd, Tb, Dy, Ho) and $R_{12}Co_6Pb$ (R=Y, La, Pr, Nd, Sm, Gd) compounds.

agreement with the behaviour of the atomic radii of the respective rare earth metals. The unit cell volumes for Co-based compounds are smaller than those of the respective Ni-based ones. The calculated density of the compounds are in good agreement with the atomic masses of the rare earth metals and cell volumes of the respective compounds.

The unit cell parameters of the $R_{12}M_6Pb$ compounds are close to the respective $R_{12}M_6In$ ones [3] (R is a rare earth metal, M is Co or Ni).

Acknowledgements

Dr Lubomir Gulay is grateful to the Śniadecki Brothers Foundation for the financial support of his research project in W. Trzebiatowski Institute of Low Temperature and Structure Research, Polish Academy of Sciences.

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