Intermetallics 38 (2013) 14–18

Contents lists available at SciVerse ScienceDirect

Intermetallics

journal homepage: www.elsevier.com/locate/intermet

Rare-earth rich indides RE_8CoIn_3 (RE = Y, Dy–Tm, Lu)

M. Dzevenko [a,*], I. Bigun [a,b], M. Pustovoychenko [a], L. Havela [b], Ya. Kalychak [a]

[a] Department of Analytical Chemistry, Ivan Franko National University of Lviv, Kyryla and Mefodia Str. 6, UA-79005 Lviv, Ukraine
[b] Department of Condensed Matter Physics, Charles University, Ke Karlovu 5, 121 16 Prague 2, Czech Republic

ARTICLE INFO

Article history:
Received 9 February 2013
Received in revised form
22 February 2013
Accepted 25 February 2013
Available online 16 March 2013

Keywords:
A. Rare-earth intermetallics
A. Ternary alloy systems
B. Crystal chemistry of intermetallics
F. Diffraction

ABSTRACT

New ternary indides RE_8CoIn_3 (RE = Y, Dy–Tm, Lu) have been prepared by arc-melting and subsequent annealing at T = 870 K. The crystal structures have been studied using X-ray powder diffraction. The RE_8CoIn_3 indides are isotypic with Pr_8CoGa_3, space group $P6_3mc$, Pearson code $hP24$: a = 10.3678(2), c = 7.0069(2) Å for Y_8CoIn_3; a = 10.3370(4), c = 6.9246(3) Å for Dy_8CoIn_3; a = 10.2856(2), c = 6.9030(2) Å for Ho_8CoIn_3; a = 10.2374(2), c = 6.8759(2) Å for Er_8CoIn_3; a = 10.1863(2), c = 6.8461(2) Å for Tm_8CoIn_3; a = 10.1168(4), c = 6.7977(4) Å for Lu_8CoIn_3. The coordination polyhedra of the RE atoms have 12-, 13- and 14-vertices. The polyhedron around the Co atom is an octahedron with one additional atom, and around the In atoms it is a strongly distorted trigonal prism with five additional atoms.

© 2013 Elsevier Ltd. All rights reserved.

1. Introduction

An interesting and distinct feature of RE-T-In (RE = rare earths, T = transition metals) systems is the existence of a large number of the ternary compounds, existing even in the rare-earth metal rich region [1]. For example, several series of such phases were reported for the RE–Co–In systems, as $RE_{12}Co_6In$ (RE = La, Pr, Nd, Sm) with the $Sm_{12}Ni_6In$ type (space group Im-3) [2], RE_6Co_2In (RE = Y, Sm, Gd–Lu) with the Ho_6Co_2Ga type (space group $Immm$) [3,4], and $RE_{14}Co_3In_3$ (RE = Y, Gd–Tm, Lu) with the $Lu_{14}Co_3In_3$ type (space group $P4_2/nmc$) [5–7]. These compounds display the typical structural chemistry of intermetallic compounds with rather small coordination numbers (CN) for all types of atom. Chemical bonding in these structures is significantly affected by numerous RE–RE contacts. The $Sm_{12}Ni_6In$- and Ho_6Co_2Ga-type representatives are characterized by isolated indium atoms. Coordination polyhedra (CP) of In are formed only of RE atoms in these structures. Other characteristic feature is transition metal dumb-bells. Generally, the distances between the d-metal atoms in such dumb-bells are smaller than the sum of the respective atomic radii in such compounds. Only the rare earths atoms are in the coordination sphere of the d-metal dumb-bells. That is why the direct T–In contacts are absent in the $Sm_{12}Ni_6In$ and Ho_6Co_2Ga structures. Practically the same situation is observed in the structure of $Er_{12}Fe_2In_3$ (space group $I4/mmm$), which does not have representatives in the cobalt systems [8]. The situation is, however, opposite in the phases with the $Lu_{14}Co_3In_3$-type. The direct Co–Co contacts do not exist in this structure, but some of the indium atoms form dumb-bells with a somewhat reduced In–In distance. Therefore the coordination sphere of Co includes besides the RE atoms also one additional atom of In. The indium atoms are coordinated either by Co and RE atoms, or by In and RE.

On the other hand, these complex structures can be also described by simple packing motifs of polyhedra [9]. The $Sm_{12}Ni_6In$ and Ho_6Co_2Ga structures can be considered as packing of icosahedra around In [InRE_{12}] and neighboring empty octahedra [ERE_6] with T-atom dumb-bells between them. The [In_2RE_{17}] clusters around the In dumb-bells can be observed in the $Lu_{14}Co_3In_3$ structure. These clusters are represented by coupled pentagonal antiprisms with sharing bases and two additional atoms. The [In_2RE_{17}] clusters are situated along the a- and b-directions and are separated by pentagonal prisms [$RERE_{10}$] in this direction.

A new rare-earth rich compound with approximate composition Er_8CoIn_3 was found in the course of investigation of the ternary isothermal section Er–Co–In at T = 870 K [10]. The analysis of the obtained X-ray powder diffraction pattern of the $Er_{67}Co_8In_{25}$ sample revealed that this compound may be isotypic to Pr_8CoGa_3 (space group $P6_3mc$, Pearson code $hP24$, a = 10.489 c = 6.910 Å) [11]. All further investigations confirmed this assumption and a series of isostructural compounds was synthesized. In the present paper we describe results of crystal structure investigation of the

* Corresponding author. Tel.: +38 032 2600389.
E-mail address: mashadzev@gmail.com (M. Dzevenko).

0966-9795/$ – see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.intermet.2013.02.020

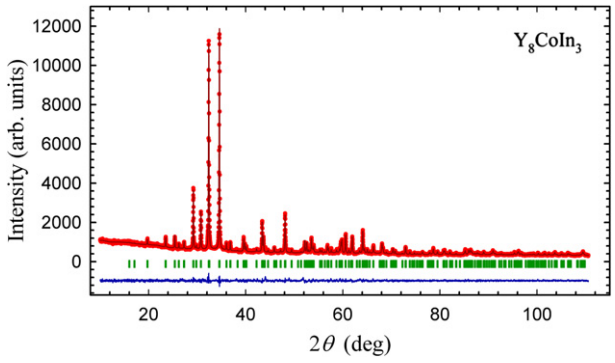

Fig. 1. Observed (·), calculated (−) and difference X-ray diffraction patterns of Y_8CoIn_3.

new series of rare-earth rich indides RE_8CoIn_3 (RE = Y, Dy–Tm, Lu) and a crystallographic analysis of their structure.

2. Experimental

Starting materials for the preparation of the samples were ingots of the rare earth metals, cobalt, and indium tear drops, all with nominal purities better than 99.9% (Johnson Matthey Co.). Ten samples of the composition RE_8CoIn_3 (RE = Pr, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu, Y) were synthesized by arc-melting of the metals under an argon atmosphere (pressure 0.7–0.8 atm). The argon gas purified by melting of titanium sponge prior to the sample fabrication. Each sample was re-melted twice to ensure homogeneity. The weight losses were smaller than what would correspond to 1 at.% of each constituent. The samples were subsequently wrapped into tantalum foil and sealed in evacuated silica tubes. A heat treatment, performed at T = 870 K for two months, was followed by quenching in cold water without breaking the tubes. After annealing no reaction with tantalum was observed. The RE_8CoIn_3 indides were obtained as silvery buttons with metallic luster and are stable in air.

X-ray powder diffraction data were collected on an automatic STOE STADI P diffractometer with a linear PSD detector (transmission mode, $2\theta/\omega$-scan; CuKα_1-radiation, curved germanium [1 1 1] monochromator; 2θ-range $6.0 \le 2\theta \le 124.5^\circ$ 2θ with step 0.015° 2θ; PSD step 0.480° 2θ, scan time 250 s/step). The value of the linear absorption coefficient was estimated from the logarithmic ratio between the primary beam intensity and its intensity after passing through background and measured samples. A preliminary data processing, X-ray profile and phase analysis were performed using the STOEWinXPOW (version 2.21) program package [12]. The crystal-structure refinement was carried out using the Fullprof software [13].

Table 2
Atomic and thermal parameters for RE_8CoIn_3 (RE = Dy–Tm, Lu, Y) compounds.

Atom	Wyckoff site	x	y	z	B_{iso}, Å^2
Y_8CoIn_3					
Y1	6*c*	0.4663(2)	−*x*	0.018(2)	0.8(1)
Y2	6*c*	0.8234(4)	−*x*	0.227(2)	1.2(1)
Y3	2*b*	1/3	2/3	0.407(2)	0.9(2)
Y4	2*a*	0	0	0[a]	1.4(1)
Co	2*b*	1/3	2/3	0.790(4)	0.6(2)
In	6*c*	0.1636(4)	−*x*	0.265(2)	1.1(1)
Dy_8CoIn_3					
Dy1	6*c*	0.4665(4)	−*x*	0.011(5)	0.3(1)
Dy2	6*c*	0.8244(9)	−*x*	0.225(6)	0.8(2)
Dy3	2*b*	1/3	2/3	0.394(5)	0.6(2)
Dy4	2*a*	0	0	0[a]	0.3(1)
Co	2*b*	1/3	2/3	0.791(8)	0.7(2)
In	6*c*	0.1642(9)	−*x*	0.260(6)	0.7(2)
Ho_8CoIn_3					
Ho1	6*c*	0.4665(2)	−*x*	0.006(2)	1.6(1)
Ho2	6*c*	0.8212(4)	−*x*	0.212(2)	1.1(2)
Ho3	2*b*	1/3	2/3	0.394(2)	1.5(1)
Ho4	2*a*	0	0	0[a]	1.6(2)
Co	2*b*	1/3	2/3	0.790(4)	0.3(1)
In	6*c*	0.1634(4)	−*x*	0.247(2)	0.4(1)
Er_8CoIn_3 [10]					
Er1	6*c*	0.4676(2)	−*x*	0.016(2)	0.7(1)
Er2	6*c*	0.8233(4)	−*x*	0.222(2)	0.6(1)
Er3	2*b*	1/3	2/3	0.398(2)	0.7(1)
Er4	2*a*	0	0	0[a]	0.8(1)
Co	2*b*	1/3	2/3	0.796(3)	1.4(5)
In	6*c*	0.1637(6)	−*x*	0.258(2)	1.2(2)
Tm_8CoIn_3					
Tm1	6*c*	0.4671(2)	−*x*	0.014(2)	0.8(1)
Tm2	6*c*	0.8224(4)	−*x*	0.223(2)	0.5(1)
Tm3	2*b*	1/3	2/3	0.398(2)	0.4(1)
Tm4	2*a*	0	0	0[a]	0.4(1)
Co	2*b*	1/3	2/3	0.790(4)	0.7(2)
In	6*c*	0.1633(4)	−*x*	0.260(2)	0.9(2)
Lu_8CoIn_3					
Lu1	6*c*	0.4673(6)	−*x*	0.028(6)	0.6(2)
Lu2	6*c*	0.8218(9)	−*x*	0.233(8)	0.7(2)
Lu3	2*b*	1/3	2/3	0.398(8)	0.4(1)
Lu4	2*a*	0	0	0[a]	0.4(1)
Co	2*b*	1/3	2/3	0.790(7)	0.8(2)
In	6*c*	0.1663(8)	−*x*	0.269(4)	0.9(3)

[a] Fixed coordinate.

Table 1
Experimental details and crystallographic data for RE_8CoIn_3 (RE = Dy–Tm, Lu, Y) compounds.

Compound	Y_8CoIn_3	Dy_8CoIn_3	Ho_8CoIn_3	Er_8CoIn_3 [10]	Tm_8CoIn_3	Lu_8CoIn_3[a]
Mr, g/mole	1114.63	1703.39	1722.83	1741.46	1754.86	1573.49
D_{cal}, g/cm^3	5.68	8.83	9.05	9.27	9.47	9.94
Lattice parameters						
a, Å	10.3678(2)	10.3370(4)	10.2856(2)	10.2374(2)	10.1863(2)	10.1168(4)
c, Å	7.0069(2)	6.9247(3)	6.9030(2)	6.8759(2)	6.8461(2)	6.7977(4)
V, Å^3	652.27(2)	640.79(5)	632.45(2)	624.08(2)	615.19(2)	602.53(6)
Absorption correction, μR_{eff}	1.48	2.00	1.25	1.37	2.26	0.60
Profile parameters *U*, *V*, and *W*	0.013(8), 0.012(8), 0.010(2)	0.017(9), 0.016(9), 0.016(5)	0.033(7), 0.006(2), 0.012(2)	0.018(7), 0.026(6), 0.007(2)	0.028(7), 0.013(6), 0.013(2)	0.07(2), 0.02(1), 0.013(6)
Asymmetry para-meters P1 and P2	0.062(4), 0.019(2)	0.055(8), 0.013(2)	0.014(6), 0.016(2)	0.038(6), 0.014(2)	0.027(4), 0.012(2)	0.017(9), 0.008(3)
Texture parameter [001]	0.041(5)	–	0.031(6)	0.038(5)	–	–
R_P, %	3.80	4.10	4.04	4.34	5.22	5.76
R_{wp}, %	5.03	4.91	5.57	4.89	6.75	7.52
R_F, %	3.78	7.31	3.76	2.53	3.60	5.74
R_{Bragg}, %	4.08	6.79	3.80	2.92	3.90	4.92

[a] – additional phase $Lu_{14}Co_3In_3$ (own str. type; space group $P4_2/nmc$; a = 9.3193(4), c = 22.499(2) Å; V = 1954.0(2) Å^3; weight fractions of phases = 33.4%; R_F = 5.52%; R_{Bragg} = 7.60%).

Download English Version:

https://daneshyari.com/en/article/1600320

Download Persian Version:

https://daneshyari.com/article/1600320

Daneshyari.com