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ISOTHERMAL SECTION OF THE Li-Yb-Si PHASE DIAGRAM AT 470K

Abstract: The isothermal section of the Li-Yb-Si system at 470 K has been investigated by X-ray phase analysis. The crystal structures of four ternary compounds formed have been determined. *

The isothermal section of the Li-Yb-Si system at 470 K has been investigated by X-ray phase analysis .Four ternary compounds were found. Crystal structures were determined for the LiYbSi compound (ZrNiAl structure type) by the powder method and for the $Li_{0.3}YbSi_{1.7}$ compound (AlB_2 structure type) by the single crystal and powder method.

The interaction of lithium with itterbium and silicon over the whole range of concentrations has not yet been studied.The Li-Si binary systems have been accepted as given by [1].Crystallographic parameters for the compounds, existing in Li-Si and Yb-Si systems were taken from [2], they are shown in Table 1.

Table 1
Crystallographic parameters for the compounds of Yb-Si and Li-Si systems

Compound	Structure type	Space group	a, nm	b, nm	c, nm
$Li_{22}Si_5$	$Li_{22}Pb_5$	F23	1,875		
$Li_{13}Si_4$	$Li_{13}Si_4$	Pbam	0,799	1,521	0,443
$Li_{14}Si_6$	Mo_2B_5	R3m	0,4435		1,8134
Li_2Si	$OsGe_2$	C2/m	0,770	0,441 $\beta = 113,4°$	0,656
$Li_{12}Si_7$	$Li_{12}Si_7$	Pnma	0,8616	1,9738	1,4341
Yb_5Si_3	Mn_5Si_3	$P6_3/mcm$	0,8215		0,6186
YbSi	BCr	Cmcm	0,4178	1,031	0,3768
Yb_2Si_3	AlB_2	P6/mmm	0,3771		0,4098
Yb_3Si_5	Pd_5Th_3	P62m	0,6512		0,4019

In this paper we present results of investigation of the isothermal section of the Li-Yb-Si system at 470 K and data of new ternary compounds which have been found.

Experimental

Isothermal section of the phase diagram of the Li-Yb-Si system has been constructed by means of X-ray phase analysis of 50 alloys prepared by arc melting in argon atmosphere.

The alloys were annealed in tanthal containers in quartz ampoules under vacuum at 470 K for 400 h.The purity of the starting metals was:Li-0.982, Yb-0.999, Si-0,9999 weight parts of the main component. The powder patterns, prepared from alloys were examined by method of X-ray photograph (camera RKD-57.3, Cr-radiation) and powder diffractometer DRON-4 (CuK_α-radiation, 0.05° step of scanning, 5-8 sec/one point speed of scanning). Single crystals obtained from alloys were examined by method of X-ray photograph (cameras RKV-86, MoK_α-radiation and CuK_α-radiation and RGNS-2 CuK_α-radiation). Lattice parameters and crystal structure refinement were calculated using LATCON and RIETVELD ANALYSES [3].

Results and discussion

The isothermal section of the phase diagram of the Li-Yb-Si system at 470 K is presented in Fig. 1 .Immiscibility gap in this system,which spreads into the ternary region up to 20 at. % Si,was observed. Four ternary compounds were found; all compounds have narrow homogeneity range. Crystallographic parameters of the ternary compounds are listed in Table 2.

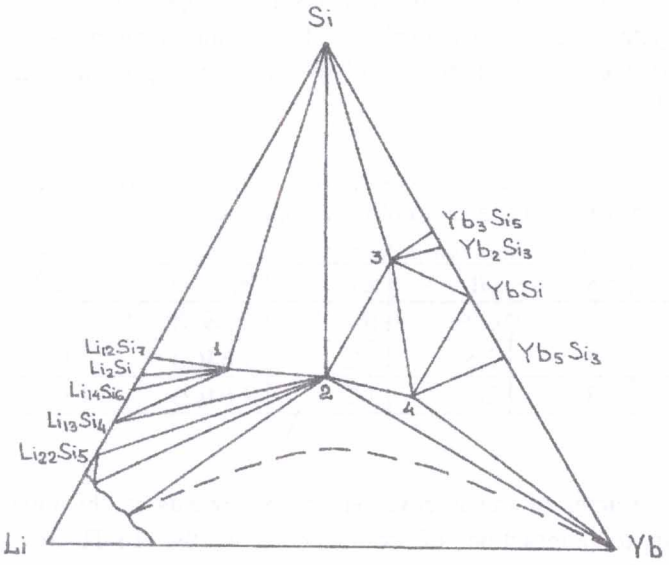

Fig. 1
Isothermal section of the Li-Yb-Si system at 470K (1 - ~$Li_{10}Yb_3Si$, 2 – LiYbSi, 3 - $Li_{0.3}YbSi_{1.7}$, 4 - ~$Li_2Yb_5Si_3$)

Table 2
Crystallographic parameters for ternary compounds of the Li-Yb-Si systems

Compound	Structure type	Space group	a, nm	c, nm
~$Li_{10}Yb_3Si$	-	-	-	-
LiYbSi	ZrNiAl	P62m	0,6515(3)	0,4096(2)
$Li_{0.3}YbSi_{1.7}$	AlB_2	P6/mmm	0,3762(1)	0,4093(1)
~$Li_2Yb_5Si_3$	-	-	-	-

Crystal structure of the LiYbSi compound was determined by the powder method. The atomic position parameters for this compound were refined to R=0.062; the corresponding values are listed in Table 3.

Table 3
Atomic parameters of the LiYbSi compound

Atom	x/a	y/b	z/c	B_i
Li	0,249(4)	0	0	2,000
Yb	0,569(1)	0	1/2	0,92(1)
Si1	1/3	2/3	0	1,59(3)
Si2	0	0	1/2	1,59(3)

Crystal structure of the $Li_{0.3}YbSi_{1.7}$ compound was determined by the single crystal and powder methods.The atomic position parameters for this compound were refined to R=0.056; the corresponding values are listed in Table 4.

Table 4
Atomic parameters of the $Li_{0.3}YbSi_{1.7}$ compound

Atom	x/a	y/b	z/c	B_i	G %
Yb	0	0	0	1,36(3)	100
Li	1/3	2/3	1/2	3,64(2)	15
Si	1/3	2/3	1/2	3,64(2)	85

Character of the interaction of components in the investigated system is similar to interaction of components in the Li-Tb-Si system, studied carlier [4]. Trigonal prismatic coordination for silicon atoms or statistic mixture of silicon and lithium characterizes compounds in both systems.It is result of the difference of atomic radii of silicon, lithium and rare earth elements. In comparison to rare earth elements, atomic radius of lithium is more similar to atomic radius of silicon; statistic mixtures of these two elements are result of this similarity.

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Izotermiczny przekrój układu Li-Yb-Si w temperaturze 470 K

Streszczenie: Za pomocą analizy rentgenowskiej badano izotermiczny przekrój układu Li-Yb-Si w temperaturze 470 K. Określono krystaliczną strukturę czterech utworzonych związków trójskładnikowych.