INTERACTION OF THE COMPONENTS IN THE Li-Al-Sb TERNARY SYSTEM AT 470 K

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The isothermal section of the Li-Al-Sb system at 470K has been investigated by X-ray phase analysis. New ternary compounds with wide and narrow homogeneity range have been obtained at 470K. Wide homogeneity range and solubility of Li for AlSb compound have been established.

INTRODUCTION

Interaction of lithium with antimony and aluminium has not been studied yet. The binary systems Li-Al, Li-Sb and Al-Sb have been accepted as given in [1]. Crystallographic characteristics for the binary compounds of these systems according to [2] are listed in Table 1.

Table 1. Crystallographic parameters for the binary compounds of the Li-Al, Li-Sb and Al-Sb systems.

Compound	Structure type	Space group	a, nm	b, nm	c, nm
Li_xAl_{1-x}	NaTl	$Fd\bar{3}m$	0.636 (x=0.5)		
Li_3Al_2	Te_3Bi_2	$R\bar{3}m$	0.4508		1.4259
Li_9Al_4	Li_9Al_4	C2/m	1.9151	0.5429	0.4499 γ=107.67°
Li_3Sb (LT)	BiF_3	$Fm\bar{3}m$	0.6572		
Li_3Sb (HT)	Na_3As	$P6_3/mmc$	0.4710		0.8326
Li_2Sb	Li_2Sb	$P\bar{6}2c$	0.7946		0.6527
AlSb	ZnS	$F\bar{4}3m$	0.61355		

EXPERIMENTAL

Isothermal section of the phase diagram of Li-Al-Sb system has been constructed by X-ray phase analysis (diffractometer DRON-2.0, FeK_α-radiation) of 68 alloys prepared by arc melting in the argon atmosphere. The alloys were annealed in tantalum containers in quartz ampoules under vacuum at 470K for 200 h and kept in inert oil. The purity of the starting metals was as follows: Li – 98.2, Al – 99.9, Sb – 99.9 weight %. Powder pattern of alloy $Li_{40}Al_{30}Sb_{30}$ was obtained by powder diffractometer SIEMENS-500 (CoK_α-radiation, 0.02° step scanning, 8-10 sec./one point speed of scanning). Lattice parameters and crystal structure refinement were calculated by of LATCON and RIETWELD ANALYSIS programs [3].

RESULTS AND DISCUSSION

The isothermal section of the phase diagram of the Li-Al-Sb ternary system at 470K is shown in Fig.1. There are two ternary compounds in

this system. The structure of ~$Li_{40}Al_{50}Sb_{10}$ compounds is not determined yet.

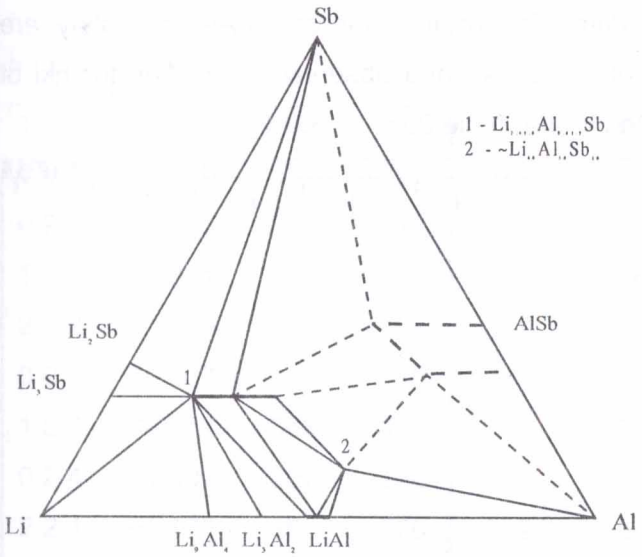

Figure 1. Isothermal section of the Li-Al-Sb system at 470K.

Change of lattice parameters of compound with wide homogeneity range $Li_{2.4+1.8}Al_{0.6+1.2}Sb$ presented in Fig.2.

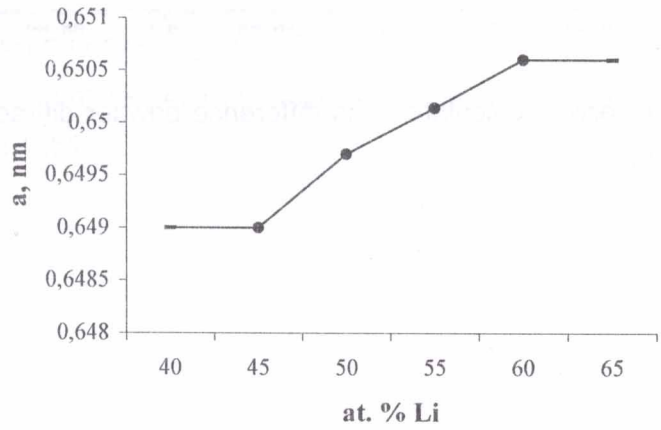

Figure 2. Change of the lattice parameter in the homogeneity range of $Li_{2.4+1.8}Al_{0.6+1.2}Sb$ compound. (• - single phase sample, - - double phase sample).

Crystal structure of this compound is refined together with structure of solid solution on the base of the AlSb compound. Observed, calculated and difference powder diffraction profiles for of $Li_{40}Al_{30}Sb_{30}$ alloy are shown in Fig 3; values of calculated and observed intensities for hkl of both phases are presented in the Table 2.

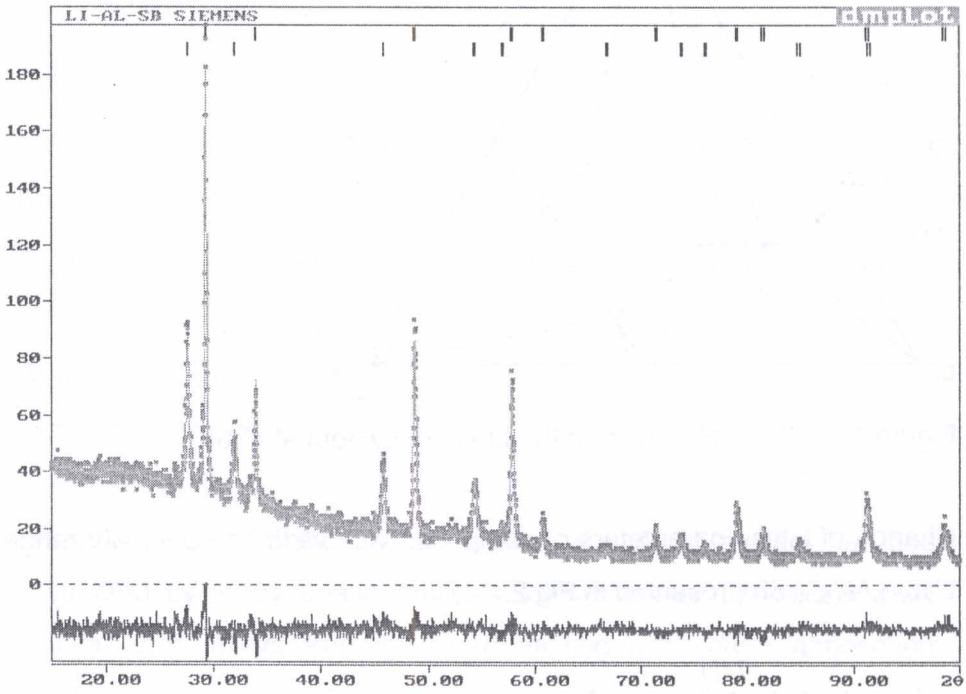

Figure 3. Observed, calculated and difference powder diffraction profiles for $Li_{40}Al_{30}Sb_{30}$.

Table 2. hkl intensities for phases of solid solution and compound with wide homogeneity range in the $Li_{40}Al_{30}Sb_{30}$ sample.

Solid solution				Compound with wide homogeneity range			
h k l	2θ	$I_{calc.}$	$I_{obs.}$	h k l	2θ	$I_{calc.}$	$I_{obs.}$
1 1 1	29.257	1428	1500	1 1 1	27.577	750	732
0 0 2	33.910	437	384	0 0 2	31.949	232	248
0 2 2	48.713	854	818	0 2 2	45.810	380	372
1 1 3	57.841	785	763	1 1 3	54.308	344	359
2 2 2	60.676	140	109	2 2 2	56.937	60	37
0 0 4	71.357	179	110	0 0 4	66.972	59	55
1 3 3	78.924	368	322	1 3 3	73.712	130	109
0 2 4	81.397	207	138	0 2 4	75.960	71	57
2 2 4	91.175	350	370	2 2 4	84.772	108	97
1 1 5	98.515	285	312	1 1 5	91.289	85	91
3 3 3				3 3 3			

Final structure of compound and solid solution was refined to R=6.89. Solid solution and compound $Li_{2.4+1.8}Al_{0.6+1.2}Sb$ are Gaysler phases and they crystallised in space groups $F\bar{4}3m$ (a=0.61347(1) nm) and $Fm\bar{3}m$ (a=0.65005(4) nm) respectively. Atomic parameters of both phases are presented in Table 3.

Table 3. Atomic parameters of phases present in the $Li_{40}Al_{30}Sb_{30}$ sample.

Atom	x/a	y/b	z/c	B_i	Occupation
AlSb					
Sb	¼	¼	¼	3.2(2)	100%
Li	0	0	0	4.0(2)	3%
Al.	0	0	0	4.0(2)	97%
Li_2AlSb					
Sb	0	0	0	3.5(1)	100%
Li	½	½	½	3.0(2)	100%
Li	¼	¼	¼	3.3(2)	28%
Al.	¼	¼	¼	3.3(2)	72%

Mechanism of formatting and boundaries of solid solution were not finally determined.

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