

## ISOTHERMAL SECTIONS OF THE Li -{Ti, V}- Bi PHASE DIAGRAMS AT 470 K

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The isothermal section of the Li-V-Bi and Li-Ti-Bi systems at 470 K has been investigated by X-ray phase analysis. There is an unmixing region which extends at about 10 at.% of Bi in the case of ternary systems. Four ternary compounds in both systems and solid solutions of the LiBi and Li<sub>3</sub>Bi binary compounds were obtained. Crystal structure were determined for the LiVBi (CdJ<sub>2</sub> structure type) and Li<sub>2</sub>TiBi (MnCu<sub>2</sub>Al structure type) ternary compounds. The solubility of V and Ti in LiBi and Li<sub>3</sub>Bi binary compounds is about 10 at.%.

The interaction of lithium with vanadium and bismuth, titanium and bismuth over the whole range of concentrations has not been studied yet. The binary systems Li-V, Li-Bi, V-Bi, Li-Ti and Ti-Bi have been accepted as given in [1,2]. Crystallographic characteristics for the binary compounds of the Li-Bi and Ti-Bi according to [2,3] are listed in Table 1.

Table 1. Crystallographic parameters for the binary compounds of the Li-Bi, Ti-Bi systems.

| Compound           | Type               | Space group or syngony | a, nm  | b, nm | c, nm  |
|--------------------|--------------------|------------------------|--------|-------|--------|
| LiBi               | AuCu               | P4/mmm                 | 0.4762 |       | 0.4256 |
| Li <sub>3</sub> Bi | BiF <sub>3</sub>   | Fm $\bar{3}$ m         | 0.6722 |       |        |
| Ti <sub>3</sub> Bi |                    | tetragonal             | 0.6020 |       | 0.8204 |
| Ti <sub>2</sub> Bi | Cu <sub>2</sub> Sb |                        | 0.4050 |       | 1.45   |

In this paper we present our results on the isothermal section of the Li-V-Bi and Li-Ti-Bi systems at 470K and data on the new ternary compounds and solid solutions.

## EXPERIMENTAL

Isothermal sections of the phase diagrams of Li-V-Bi and Li-Ti-Bi systems have been constructed by X-ray phase analysis of 40 and 42 alloys prepared by arc melting in argon. The alloys were annealed in quartz ampoules under vacuum at 470K for 400 h. The purity of the starting metals was better than 99,9 %. Powder patterns of alloys were obtained by powder diffractometer DRON-2.0 (FeK $\alpha$  - radiation, 0,02<sup>o</sup> step of scanning, 8-10 sec./one point speed of scanning). Lattice parameters and crystal structure refinement were calculated using LATCON and RIETWELD ANALYSES programs [4].

## RESULTS AND DISCUSSION

The phase diagram of the Li-V-Bi ternary system at 470K is shown in Fig.1.

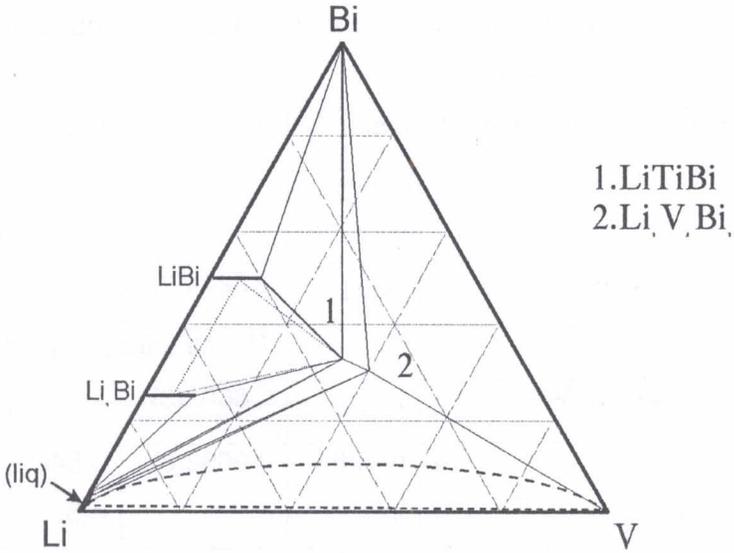


Figure 1. Isothermal section of the Li-V-Bi system at 470 K.

This system is characterized by presence of field of unmixing Li and V, which in ternary area reaches approximately up to 10 at. % of Bi. Two ternary compounds  $\text{LiVBi}$  and  $\text{Li}_3\text{V}_4\text{Bi}_3$  were found in the system. The compound  $\text{LiVBi}$  has a structural type  $\text{CdJ}_2$  (space group  $P\bar{3}m1$ ), parameters of atoms are

|      |     |     |     |
|------|-----|-----|-----|
| Bi   | 0   | 0   | 0   |
| Li+V | 1/3 | 2/3 | 1/4 |

The structure of  $\text{Li}_3\text{V}_4\text{Bi}_3$  ternary compound is not investigated. The crystallographic characteristics of ternary compounds of the Li-V-Bi system is gathered in Table 2.

Table 2. Crystallographic characteristics of ternary compounds of the Li-V-Bi and Li-Ti-Bi systems.

| Compound                                       | Structure type       | Space group, syngony | a,nm                             | b,nm      | c,nm      |
|--|----------------------|----------------------|----------------------------------|-----------|-----------|
| LiVBi  | CdI <sub>2</sub>     | P $\bar{3}$ m1       | 0.3244(1)                        |           | 0.5125(2) |
| Li <sub>3</sub> V <sub>4</sub> Bi <sub>3</sub> |                      |                      | The structure is not determinate |           |           |
| Li <sub>2</sub> TiBi                           | MnCu <sub>2</sub> Al | Fm $\bar{3}$ m       | 0.6663(3)                        |           |           |
| LiTiBi   |                      | orthorhombic         | 0.9698(6)                        | 0.8484(5) | 0.7889(4) |

One should note the limited solid solutions on the base of LiBi and Li<sub>3</sub>Bi binary compounds. The solubility of vanadium is approximately 10 at %; its mechanism concerns substitution of Li atoms by V atoms. Borders of solid solutions are shown in Fig.2.

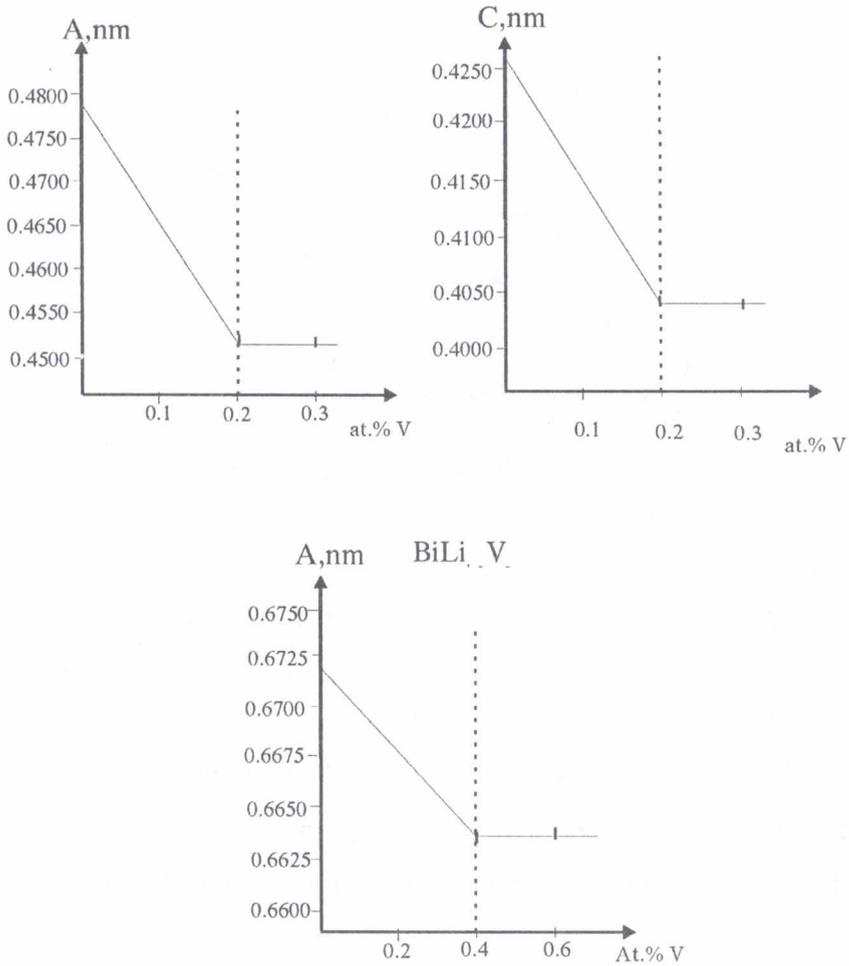


Figure 2. Change of lattice parameters for the  $\text{LiBi}_{1-x}\text{V}_x$  and  $\text{LiBi}_{3-x}\text{V}_x$  solid solutions.

The phase diagram of the Li-Ti-Bi ternary system at 470 K is shown in Fig.3.

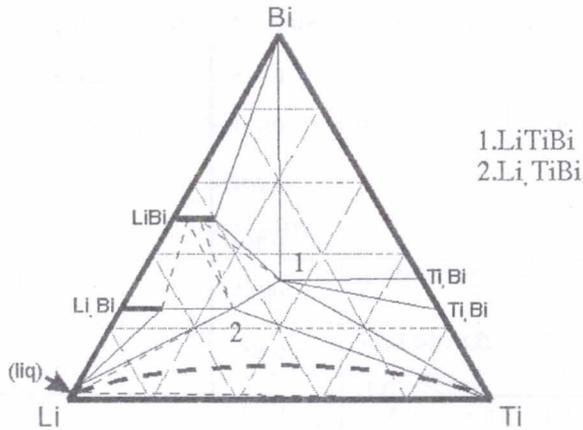


Figure 3. Isothermal section of the Li-Ti-Bi system at 470 K.

This system is characterized by presence of field of unmixing Li and Ti, which extends approximately up to 10 at % of Bi at ternary area.

Existence of two ternary compounds  $\text{LiTiBi}$  and  $\text{Li}_2\text{TiBi}$  is discovered in the system.

The  $\text{Li}_2\text{TiBi}$  compound is in accordance with Gaisler's phases. It is crystallizing in structure type of  $\text{MnCu}_2\text{Al}$  (space group  $\text{Fm}\bar{3}\text{m}$ ). Parameters of atoms of  $\text{Li}_2\text{TiBi}$  compound are shown in Table 3.

Table 3. The atomic parameters of  $\text{Li}_2\text{TiBi}$  ternary compound.

| Atom |      | x/a           | y/b           | z/c           | $B_i$  |
|------|------|---------------|---------------|---------------|--------|
| Li   | 8(c) | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | 2.0    |
| Ti   | 4(b) | $\frac{1}{2}$ | 0             | 0             | 1.4(2) |
| Bi   | 4(a) | 0             | 0             | 0             | 1.1(3) |

The  $\text{LiTiBi}$  ternary compound is in accordance with to orthorhombic syngony. Full determination of a crystal structure of the  $\text{LiTiBi}$  compound has been impossible, because the single-crystal samples decompose during the investigation. The crystallographic characteristics of ternary compounds of the Li-Ti-Bi system are gathered in Table 2.

There are observed limited solid solutions, on the base of  $\text{LiBi}$  and  $\text{Li}_3\text{Bi}$  binary compounds. The solubility of titanium equals approximately 10 at %; its mechanism concerns substitution of Li atoms by Ti atoms. Borders of solid solutions are shown in Fig.4.

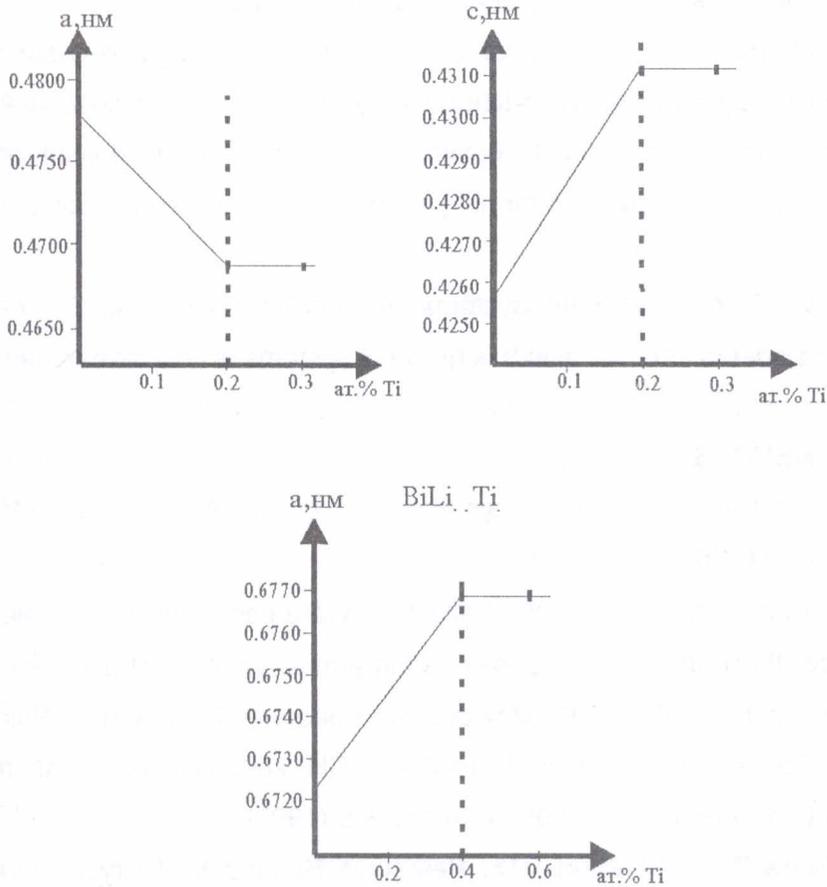


Figure 4. Change of lattice parameters for the  $\text{LiBi}_{1-x}\text{Ti}_x$  and  $\text{LiBi}_{3-x}\text{Ti}_x$  solid solutions.

Explored system comparison shows that interaction of components in them is very probable. In both systems, fields of unmixing Li and V, Li and Ti, solid solutions of substituting on the base binary intermetallids  $\text{LiBi}$  and  $\text{Li}_3\text{Bi}$ , will be formed in the case of 2 ternary compounds. Formation of the

solid solutions, is obviously stipulated by the small difference between atomic radii of Li and V, and Li and Ti.

Comparison of Li-V-Bi and Li-Ti-Bi systems with earlier studied Li-T-X (T – rare earth metal, X - p-element) systems, shows a single similarity – formation of a small quantity of a ternary compound.

Resemblance of interaction of components in investigated systems is shown by systems Li-{Ti,V}-{Ge,Si} only. There are also observed: the field of unmixing of Li and Ti, Li and V; formation of solid solutions on the base of binary phases and forming a small quantity of ternary compounds [5,6].

Li-{Ti,V}-M (M – p-element) systems are insufficiently studied. The nature of components interaction in this group of systems is now researched.

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