

## STRUCTURE OF SOLID SOLUTIONS BASED ON $Bi_2B^{VI}_3$ AND $Sb_2B^{VI}_3$ ( $B^{VI}$ - Se, Te)

Xolmatova Ruxshona Musinjon qizi

Fergana State University, 3rd year student of Physics

### ABSTRACT

This article presents the crystal lattice structure of  $Bi_2B^{VI}_3$  and  $Sb_2B^{VI}_3$  ( $B^{VI}$  - Se, Te) solid alloys, changes in their parameters under a certain temperature.

**Key words:** solid alloy, solid solution, stoichiometric composition, crystal lattice, crystal lattice parameters

### АННОТАЦИЯ

В статье представлена структура кристаллической решетки твердых сплавов  $Bi_2B^{VI}_3$  и  $Sb_2B^{VI}_3$  ( $B^{VI}$  - Se, Te) изменение их параметров при определенной температуре.

**Ключевые слова:** твердый сплав, твердый раствор, стехиометрический состав, кристаллическая решетка, параметры кристаллической решетки.

### ANNOTATSIYA

Ushbu maqolada  $Bi_2B^{VI}_3$  va  $Sb_2B^{VI}_3$  ( $B^{VI}$  - Se, Te) qattiq qotishmalarning kristall panjara tuzilishi, ma'lum harorat ostida ularning parametrlari o'zgarishlari keltirilgan.

**Kalit so'zlar:** qattiq qotishma, qattiq eritma, stexiometrik tarkib, kristall panjara, kristall panjara parametrlari.

One of the pressing issues in the world is the implementation of the mutual conversion of heat and electricity through thermoelectric materials with high efficiency without harming the atmosphere in obtaining environmentally friendly electricity. Ushbu  $Bi_2B^{VI}_3$  va  $Sb_2B^{VI}_3$  ( $B^{VI}$  - Se, Te) Among the chalcogenides that are components of solid solutions based on  $Bi_2B^{VI}_3$  and  $Sb_2B^{VI}_3$  ( $B^{VI}$  - Se, Te) bismuth telluride has been studied in the most detail. Thermoelectric materials based on bismuth antimony telluride and selenide with high thermoelectric properties and characteristics are important in creating thermoelectric devices. Such thermoelectric materials are widely used in generators, refrigerators, thermostats, air conditioners and other devices to convert heat energy directly into electricity. Therefore, solid solutions based on bismuth telluride ( $Bi_2Te_3$ ) have the best thermoelectric properties in the temperature range of 200-600 K.

$Bi_2Te_3$  forms continuous isomorphous solid solutions with  $Bi_2Se_3$  and  $Sb_2Te_3$ . A number of conditions must be met for this:

1) initial compounds must belong to the same symmetry class and have lattices with similar parameters;

2) atoms replacing each other should not differ greatly in size and be similar in chemical properties.

All these conditions are well fulfilled for Bi<sub>2</sub>Te<sub>3</sub> Bi<sub>2</sub>Se<sub>3</sub> and Sb<sub>2</sub>Te<sub>3</sub> (Table 1).

Table 1. Space group and lattice parameters of Bi<sub>2</sub>Te<sub>3</sub>, Sb<sub>2</sub>Te<sub>3</sub> and Bi<sub>2</sub>Se<sub>3</sub> at T= 300 K

Compound Lattice	Space group	parameters, Å	
Bi <sub>2</sub> Te <sub>3</sub> [35]	$D_{3d}^5(R\bar{3}m)$	4,3835	30,487
Sb <sub>2</sub> Te <sub>3</sub> [51]	$D_{3d}^5(R\bar{3}m)$	4,275	30,490
Bi <sub>2</sub> Se <sub>3</sub> [50]	$D_{3d}^5(R\bar{3}m)$	4,134	28,546

Covalent radii for Se, Bi, Te and Sb are respectively: 1.17; 1.51; 1.37 and 1.41 Å. In Bi<sub>2</sub>Te<sub>3</sub> - Sb<sub>2</sub>Te<sub>3</sub> solid solutions, Bi sites are replaced by Sb atoms.



In Bi<sub>2</sub>Te<sub>3</sub> - Bi<sub>2</sub>Se<sub>3</sub>, the Se atom is primarily located in Te<sup>(1)</sup> and Te<sup>(2)</sup> and forms the following chains:



Lattice parameters of Bi<sub>2</sub>Te<sub>3</sub> - Sb<sub>2</sub>Te<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub> - Bi<sub>2</sub>Se<sub>3</sub> - were measured in [42, 46, 48, 50]. Data for the first solid solution are shown in Figure 1, and for the second - in Figure 2. The parameter a obeys Wegart's rule in both cases.

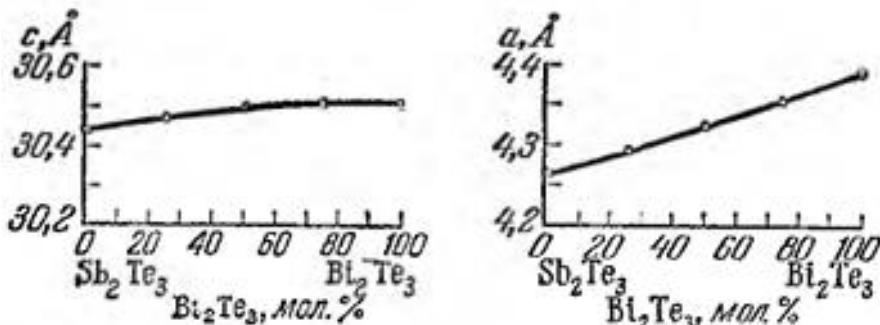


Figure 1. Variation of a, c parameters depending on the composition of the Bi<sub>2</sub>Te<sub>3</sub> - Sb<sub>2</sub>Te<sub>3</sub> solid solution system.

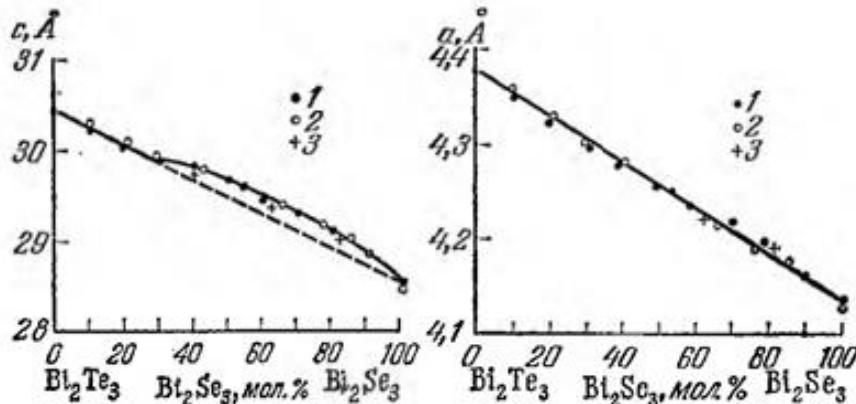


Figure 2. Dependence of parameters  $a$  and  $c$  on composition in  $\text{Bi}_2\text{Te}_3$  -  $\text{Bi}_2\text{Se}_3$  solid solution: 1 - hardened samples; 2, 3 - single crystals grown at a speed of 1.2 and 0.2 mm/h, respectively.

It decreases when going from  $\text{Bi}_2\text{Te}_3$  to  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$ , mainly because the substituent atoms (Se and Sb) are smaller compared to the matrix atoms (Te and Bi).

The  $c$  parameter changes in a more complex way depending on the composition of the solid solution. So, for example, in  $\text{Bi}_2\text{Te}_3$  -  $\text{Bi}_2\text{Se}_3$ ,  $c$  decreases linearly only up to 30 mol%  $\text{Bi}_2\text{Se}_3$ , after which a deviation from Vegart's law is observed (Fig. 3). In this solution, Se replaces Te(2) until the composition  $\text{Bi}_2\text{Te}_2\text{Se}$ , and only then Te(1).

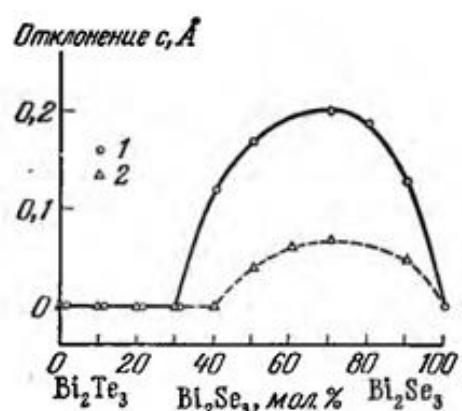


Figure 1.9. Deviation from Vegart's law for parameter  $c$  in  $\text{Bi}_2\text{Te}_3$  -  $\text{Bi}_2\text{Se}_3$  solid solution: 1 - data obtained from work; 2 - [48].

A deviation from Vegart's law in parameter  $c$  is observed near  $\text{Bi}_2\text{Te}_2\text{Se}$ . This may be due to changes in van der Waals interactions between individual quintets. It is known that such an interaction is stronger between identical systems ( $\text{Te}(1)$  -  $\text{Te}(1)$ ) or  $\text{Se}$  -  $\text{Se}$ ) than between dissimilar systems ( $\text{Te}(1)$  -  $\text{Se}$ ) is stronger. If this assumption is correct, the maximum deviation from Vegart's law should be for a  $\text{Bi}_2\text{Se}_3$  composition of 67 mol%, which corresponds to a 50% to 50% mixture of Te and Se atoms in the  $\text{Te}(1)$  layers. will come. This is well confirmed by experience (see Figure 1.9).

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