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CRYSTAL STRUCTURE OF SECONDARY COMPOUNDS

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Abstract: In this article, it is explained that as a result of the melting of secondary alloys, the formation of a continuous series of solid solutions and the formation of parallel layers, the atoms of the layer and the planar hexagonal lattice formed by them. Among the chalcogenides that are components of these solid solutions, bismuth telluride has been studied in the most detail. This is because, firstly, bismuth telluride itself has very high thermoelectric parameters and was widely used as a working material in early models of thermoelectric devices.

Among the chalcogenides that are components of these solid solutions, bismuth telluride has been studied in the most detail. This is because, firstly, bismuth telluride itself has very high thermoelectric parameters and was widely used as a working material in early models of thermoelectric devices. Secondly, it was possible to make it p- and n-type with a doping agent. Finally, bismuth telluride was easy to prepare in the form of very perfect single crystals. There is no single point of view on the regulation of processes in these considered solid solutions, and there is no detailed information on the shift in stoichiometry. This is explained by the multicomponent nature of materials and the presence of various interatomic interactions in the crystal lattice.

Keywords: hexagonal elementary cell, van der Waals forces, atom, ion, crystal lattice, solid solution, chalcogenide

Introduction

One of the urgent 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. 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 (Bi2Te3) have the best thermoelectric properties in the temperature range of 200-600 K. As the thermoelectric efficiency increases, the energy characteristics of devices improve. The values of α, σ and χ, in turn, depend on the main physical parameters of the substance. For example, lattice thermal conductivity χp, mobility μ and effective mass of charge carriers m^*, and these parameters are included as a first approximation. The structure of thermocouple branches made of materials based on Bi2Te3 also has a significant effect on thermoelectric efficiency. This is due to the significant anisotropy of electrical and thermal conductivity characteristic of these materials, as well as the tendency to form uniformity of concentration during the crystallization process.

It was shown that the system under consideration forms a continuous series of solid solutions. Based on this system, he created an efficient thermoelectric material. Initially, 50 mol of alloy was used. 50 mol % Bi2Te3+ 50 mol.% Sb2Te3, then the composition 26 mol.%

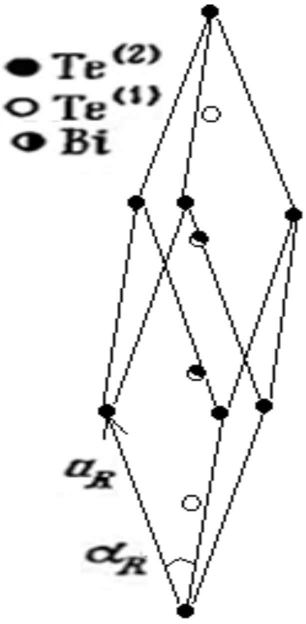

Fig. 1.Rhombohedral

Bi2Te3 + 74 mol showed high efficiency. % Sb2Te3 + 3 wt.% . Te (flow above stoichiometry). With some variations of the Bi2Te3 component (from 20 to 30 mol%), it is still used as p-junctions of thermocouples.

When synthesizing the thermoelectric material for the n-network of the thermocouple based on Bi2Te3 - Bi2Se3, good thermoelectric properties were demonstrated with a solid solution of 80 mol% Bi2Te3 + 20 mol% Bi2Se3.

Thus, since 1956, solid solutions of Bi2Te3 with Sb2Te3 and Bi2Se3 have become the main materials for cooling thermocouples.

Method and material

Despite the fact that Vi2Te3 and its solid solutions are highly anisotropic, when many measurements were made on polycrystalline samples, which are often used in thermoelectric devices, the study of polycrystals still made it possible to obtain a number of useful information about their properties. For example, determining the effect of various mixtures, determining some physical quantities that do not have a strong anisotropy of their properties by order of magnitude.

We used the technology of melting under inert gas pressure to obtain such hard alloys. Because a number of disadvantages of other methods have been observed, the effect on the electrophysical parameters of the obtained material. In order to increase the thermoelectric efficiency of thermoelectric materials obtained under inert gas pressure, it is necessary to correctly select the composition and operating parameters of materials based on Bi2Te3 and Bi2Se3. In the process of obtaining secondary thermoelectric materials, the chalcogenides must be infinitely dissolved in each other, forming a continuous series of solid solutions. In this case, the compounds should belong to the same symmetry class and have lattices with close parameters, the atoms that replace each other should not differ much from each other in terms of size, and their chemical properties should be close.

Describing the structure of the compound Bi2Te3 as rhombohedral with space group D53d($R\bar{3}m$) and parameters

$$a_R=10{,}45\ \text{Å} \qquad \propto_R=24{,}8' \qquad (1)$$

Figure 1 shows the rhombohedral unit cell of Bi2Te3. At 300 K of well-annealed powders with stoichiometric composition

$$a_R=10{,}477\ \text{Å} \qquad \propto_R=24°9'32'' \qquad (2)$$

will have size.

It is often more convenient to describe the structure of Bi2Te3 using a hexagonal rather than a rhombohedral unit cell. The parameters a and c of such a cell can be written as a_R and ∝_R using the conversion formulas

$$a=2a_R \sin(\propto/2), \qquad c=\sqrt{3}\, a_R (1+2\cos\propto)^{1/2} \qquad (3)$$

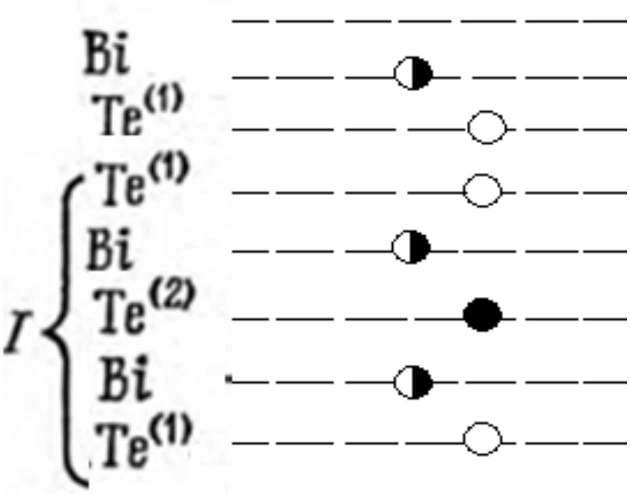

Fig.2. Arrangement of atoms in the Bi_2Te_3 lattice quintet

Combining (2) and (3), we obtain for the parameters a and c Bi2Te3

$$a=4{,}3835\pm0{,}0005\ \text{Å} \qquad c=30{,}487\pm0{,}001\ \text{Å} \qquad (4)$$

The structure of Bi2Te3 can be represented as a set of complex layers - quintets, perpendicular to the axis of symmetry of the third order (axis c in the hexagonal lattice). There are three such quintes in a hexagonal cell. Each quintet consists of five simple layers (Figure 2). The atoms of a single layer are identical and form a flat hexagonal lattice. Layers alternate in sequence

-Te(1) - Bi- Te(2)- Bi - Te(1)-

In this case, the atoms of each subsequent layer are located on the centers of the triangles formed by the atoms of the previous layer (close hexagonal packing).

Due to the layered structure, Bi2Te3 (0001) is easily cracked along the planes.

Te(2)atoms have six Bi atoms as nearest neighbors (three from each adjacent layer). Te(1), on the one hand, is bonded to three Bi atoms, and on the other hand, to three Te(1) atoms. Thus, there are two significantly different locations for tellurium atoms in the lattice. Accordingly, Bi has three neighbors Te(2) and three Te(2).

In mixed conductivity, the value of Z also depends significantly on the band gap and the ratio of the parameters μ0 (m*/m0)3/2 for electrons and holes. The maximum value of Z corresponds to a certain concentration of charge carriers, which is achieved by introducing dopants or changing the composition of the material relative to the stoichiometric one.

The structure of the branches of thermocouples made of materials based on Bi2Te3 also has a significant impact on the thermoelectric efficiency. This is due to the significant anisotropy of electrical and thermal conductivity inherent in these materials, as well as the tendency to form concentration inhomogeneities during crystallization.

Conclusion

When obtaining thermoelectric materials under inert gas pressure, it is necessary to study the internal structure of elements, that is, the structure of crystal lattices, the effect of chalcogens included in secondary thermoelectric materials on electrophysical parameters, and their effect on the crystal lattice. When obtaining thermoelectric materials under inert gas pressure, it is necessary to study the internal structure of the elements, that is, the structure of the crystal lattices, and the effect of chalcogens introduced into secondary thermoelectric materials on the electrophysical parameters, in order to study their effect on the crystal lattice.

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