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Theoretical models of ordered alloys of Bi-Sn-Te based thermoelectric materials

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A comprehensive approach has been developed for constructing theoretical models of Bi-Sn-Te based ordered alloys. Calculations of effective radii, redistribution of electron density and dissociation energy of nonequivalent hybrid orbitals (NHO) in the Bi-Sn-Te system depending on interatomic distances have been presented. A scheme for improving the technology of switching the thermoelement legs, taking into account the peculiarities of the chemical bond, has been proposed.

Keywords: theoretical models, chemical bond, effective radii, electron density, state diagrams.

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Introduction

Bismuth telluride is considered the most studied thermoelectric material [1]. However, despite many years of research into its physicochemical properties, many important questions remain unclear, and the theoretical explanation of many empirical dependencies is associated with a revision of views on the problem of interatomic interactions [2].

The issue of studying the problems of synthesizing new thermoelectric materials based on tellurides remains relevant. At the same time, the search for new promising materials is increasingly reduced to the need to study multicomponent systems in which solid phases of variable composition and structure are formed. The nature of the chemical bond in such systems varies widely and is associated with the features of phase diagrams and phase transformations both in the solid state and in melts [3].

The issue of the technology of switching the branches of a thermoelement, which significantly affects the quality of the thermoelectric module, also remains relevant. Switching is a complex technological process: it is necessary to obtain inseparable contact connections between branches of p- and n-type conductivity compatible in terms of physicochemical properties with a minimum of losses at electrical and thermal junctions with high stability, sufficient mechanical strength and resistance to thermal changes [4].

One of the switching methods is soldering with solders containing tin and lead. Over time, they diffuse into the thermoelectric material and deteriorate its properties. Therefore, there is a need to reduce the diffusion of solder into the semiconductor material of the thermoelement branches. For this, anti-diffusion coatings are placed between the solder and the thermometric material, which prevent the diffusion of chemical elements from the plate material into the semiconductor. The application of switching layers to the surface of semiconductors can be carried out by various methods: chemical, galvanic and their varieties. This paper proposes a scheme for improving the technology of switching the thermocouple branches, taking into account the features of the chemical bond of the initial components of the system under study.

It should also be noted that when studying complex systems, the classical scheme of dividing them into a sum of one-sided experiments no longer reveals the conditions for the appearance of the required properties, and there still does not exist a consistent theory of phase transformations taking the chemical bond into consideration.

New methods and approaches to solving such problems are being sought. Their solution is possible by combining the results of experimental and theoretical studies. The basis of such synthesis, according to [5], is the energy approach. The combination of the electronic, vibrational and configurational components of energy enabled calculating the ordering processes in alloys by statistical methods; the regularities of the formation of short-range order of chemical bonds in melts by quantum-chemical methods; the redistribution of electron density and dissociation energy of non-equivalent chemical bonds by methods of microscopic theory using solutions of inverse problems and molecular models [6].

This work is an extension of the works [2-6] and is devoted to solving the problems of switching from the position of chemical bonding. This allows establishing the regularities of contact formation at the molecular level; optimizing the need to reduce the diffusion of solder into the semiconductor material of the thermoelement legs.Moreover, in the absence of a strict microscopic theory of disordered systems, the results obtained expand the empirical base of existing theoretical developments.

I. Theoretical models of phase equilibria of Bi-Sn-Te

When constructing the phase region distribution scheme of Bi-Sn-Te, it was necessary to summarize the results of experimental studies of phase diagrams of Bi-Sn, Bi-Te, Sn-Te.

In this regard, in this work, phase region distribution schemes for equilibrium in the solid state are constructed and isothermal cross-sections of ternary systems Bi-Sn-Te at different temperatures are carried out, combining experimental and theoretical approaches with calculations of the interaction energy of components in ternary systems. The obtained results are presented in Figures 1-5, where the following notations are introduced:

α – solid phase based on Bi;

δ – solid phase based on Bi-Sn;

β – solid phase based on Te;

γ – solid phase based on Sn;

σ – solid phase based on Sn-Te;

λ – solid phase based on Bi-Te;

θ – solid phases based on intermediate compound Bi-Sn-Te;

L – liquid.

Fig. 1 shows a diagram of the distribution of phase regions of Bi-Sn-Te in the solid state. The division of the ternary system Bi-Sn-Te into six ordered ternary subsystems is clearly traced. This makes it possible to consider the issue of interatomic interaction both from the standpoint of phase diagrams and chemical bonding. If additional experimental data on intermediate compounds, solid solutions, and mechanical mixtures are available, the number of ordered ternary systems may be greater.

Fig. 2 shows an isothermal cross-section at a

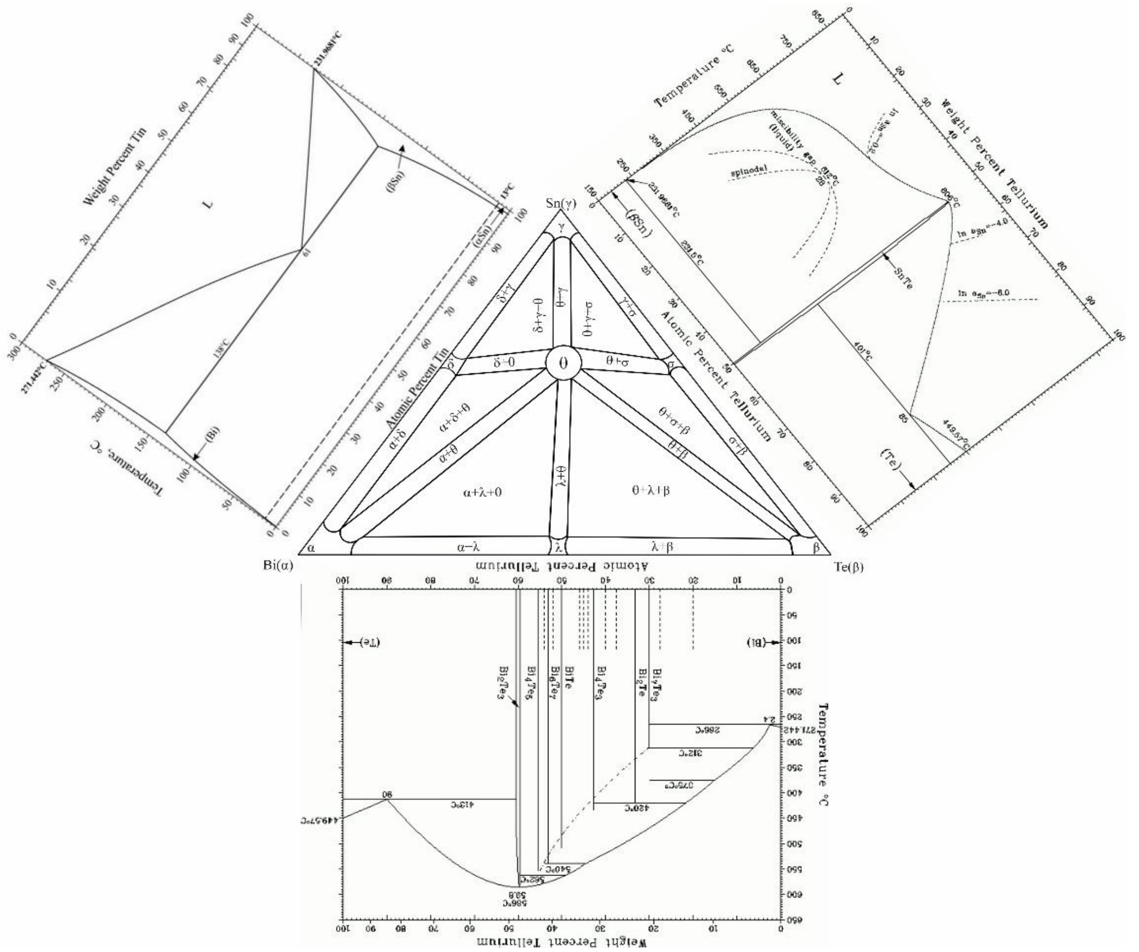


Fig. 1. Scheme of distribution of solid phase equilibrium regions in the solid state of Bi-Sn-Te.

temperature of t=150°C, which is lower than the melting point of Bi, Sn, Te and at the same time higher than the temperature of the first eutectic of the Bi-Sn system (139°C). The two-phase equilibrium (L+γ); (L+α) is carried out by the primary crystals α and γ and the liquid, as well as by δ-crystals based on compounds (Bi_nSn_m) and the liquid and form a conode triangle (L+δ+θ).

Fig. 3 shows an isothermal cross-section of Bi-Sn-Te at a temperature of t=200°C, which is lower than the melting point of the initial components, but higher than in the previous case. Most of the Bi-Sn cross-section is occupied by the liquid. Unlike the previous case, the Bi-Sn cross-section contains conode triangles with equilibrium phases (L+α+θ); (L+δ+θ); (L+γ+θ). At this temperature, subsystems not associated with Bi-Sn remain unchanged.

Fig. 4 shows an isothermal cross-section of Bi-Sn-Te at a temperature of t=300°C, which is higher than the melting point of Bi and Sn, but lower than the melting point of Te. In this case, the Bi-Sn cross-section is completely occupied by liquid, and the Bi-Te and Sn-Te cross-sections contain conoid triangles with equilibrium phases, which are realized by primary β crystals, as well as σ- and δ-crystals based on Bi_nSn_m compounds and liquid. Such division of ternary systems into separate sectors of binary phase diagrams makes it possible to study the fine structure of cooling and heating of individual elements depending on their environment and the processes of formation of short-range chemical bond order.

Fig. 5 shows an isothermal cross-section of Bi-Sn-Te at a temperature of t=420°C, which is higher than the melting point of Bi and Sn. The entire Bi-Sn cross-section is occupied by liquid, and on the Bi-Te and Bi-Sn diagrams, three-phase diagrams are represented by conoid triangles with phases (L+θ+β); (L+σ+θ). Thus, the given isothermal cross-sections make it possible to:

1. Establish quantitative ratios of coexisting phases and their concentrations.

2. Determine the limits of phase equilibrium in the liquid-crystal regions.

3. Predict cases of incongruent melting of chemical compounds of different compositions.

However, isothermal cross-sections alone do not yet indicate the temperatures of phase transitions of multicomponent systems. Theoretical models are needed that combine generalized experimental data with calculations of interatomic interaction of components in different phases depending on interatomic distances and increase the role of theoretical calculations in constructing phase diagrams of multicomponent systems.

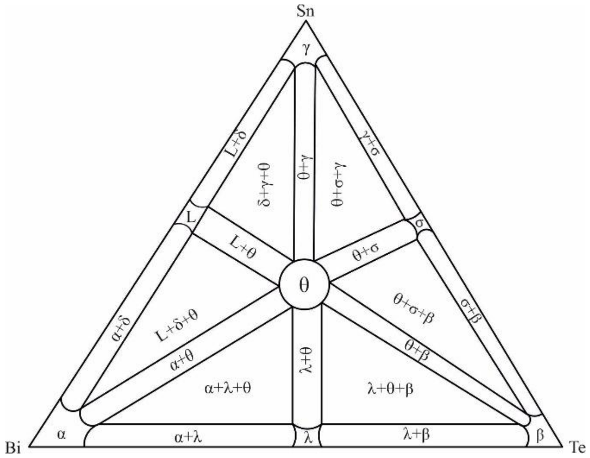


Fig. 2. Isothermal cross-section of Bi-Sn-Te at t=150°C.

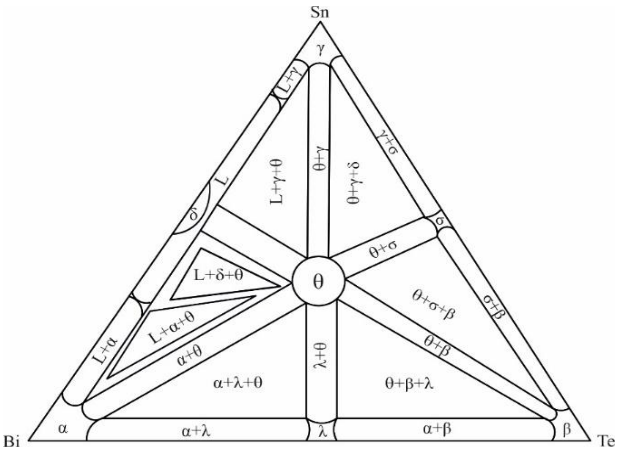


Fig. 3. Isothermal cross-section of Bi-Sn-Te at t=200°C.

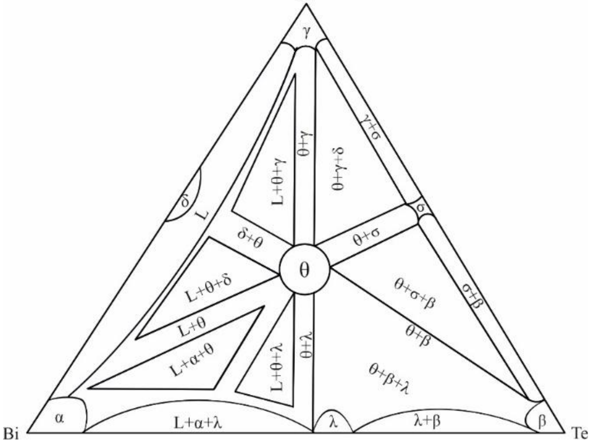


Fig. 4. Isothermal cross-section of Bi-Sn-Te at t=300°C.

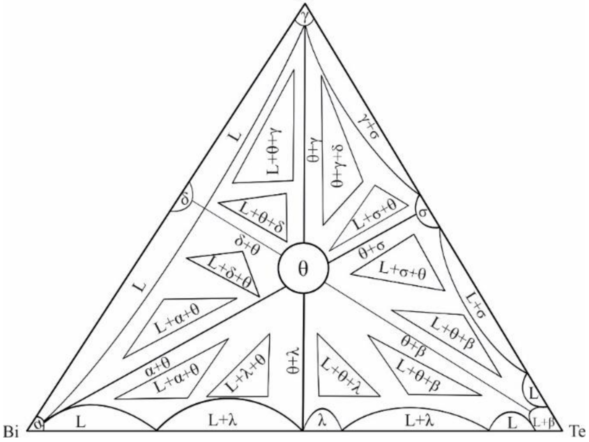


Fig. 5. Isothermal cross-section of Bi-Sn-Te at t=420°C.

II. Theoretical models of chemical bonding in ordered alloys Bi-Sn-Te

When constructing theoretical models of Bi-Sn-Te, it was necessary to summarize the results of studies of physicochemical properties and quantum laws of the dynamics of chemical bond formation by analyzing interatomic interactions in the starting components; binary systems of the starting components (Bi-Sn; Bi-Te; Sn-Te) and isothermal cross-sections of ternary systems Bi-Sn-Te at different temperatures.

Consideration of bismuth as a component of Bi-Sn-Te showed that bismuth can have different oxidation states (from -3 to +5) in compounds. In addition, in the state diagrams (Bi-Sn) and (Bi-Te), Bi behaves differently.

The state diagram (Bi-Sn) is a diagram with eutectics. The eutectic temperature is 139°C [7], which is lower than the melting point of Bi (271.4°C) and Sn (231.9°C). Moreover, solid solutions of Bi_nSn_m with a composition of Bi≤13.1% crystallize with supercooling and are supersaturated, from which Bi crystals precipitate with decreasing temperature.

The state diagram (Bi-Te) [8] is a diagram with a degenerate eutectic. Melting point of the compound Bi_2Te_3 is 586°C. The diagram also has two closely spaced eutectics: near Bi with a Te content of 2.4% and a temperature of 366°C and near Te with a Bi content of 10% and a temperature of 413°C.

The state diagram (Sn-Te) [9] is also with a degenerate eutectic. Melting point of the compound SnTe is 806°C. The diagram has two closely spaced eutectics: near Sn with a temperature of 231.5°C at the melting point of Sn of 231.9681°C and near Te with a content of 15% Sn and a eutectic temperature of 401°C at the melting point of Te of 449.57°C.

Theoretical analysis of the given empirical dependences is connected to the revision of views on the problem of interatomic interaction. For example, calculation of electron density between interacting atoms by quantum mechanical methods contradicts the fact that formation of chemical bond is accompanied by restructuring of spherical covalent electron shells of atoms and redistribution of electron density along chemical bonds.

To overcome such a contradiction generalization of the experience and traditions of statistical, crystal chemical and quantum mechanical approaches to the case of chemical bond was required [5].

Taking into account statistical regularities allowed obtaining the dependence of a number of electrons n on outer shell of the atom on Fermi radius r_F. Empirical information on the basis of crystal chemical approach can be combined by introducing the idea of unpolarized ionic radii R_{Un}.

The fact that both the functions that include the Fermi radii $r_F = f(n)$ and the equations that include R_{Un} determine the electronic configurations of interacting atoms depending on the distance and the number of bonds formed by them gave grounds to consider the concepts of the Fermi radius r_F and the unpolarized radius R_{Un} to be identical, and to denote the effective ionic radii with one symbol R_U [10].

The numerical values of electronegativity turned out to be the most useful in searching for a graphical solution to the problem of the relationship R_U and n. By fixing the position of the direct coordinates $lgR_U = f(n)$, the relationship $tg\alpha = \frac{\Delta lgR_U}{\Delta n}$ and electronegativity was found [10].

A good agreement of the complex of experimental data on various physicochemical properties of atoms and their ions with the values of R_U and $tg\alpha$ gives the postulated dependence:

$$lgR_{UA}^{x} = lgR_{UA}^{0} - xtg\alpha, \tag{1}$$

where $R_{U\text{A}}^{0}$ is radius of atoms A in an unexcited state, and x is valence.

Since the equations of the system of ionic radii describe the change in R_U of atoms when the number of electrons in the orbitals of each changes, assuming equality of the absolute values of the charges of the interacting atoms, dependence (1) takes the form of a system of equations:

$$lgR_{UA}^{+x} = lgR_{UA}^{0} - xtg\alpha_{\text{A}}, \tag{2}$$

$$lgR_{U\text{B}}^{-x} = lgR_{U\text{B}}^{0} + xtg\alpha_{\text{B}}, \tag{3}$$

$$d_1 = R_{UA}^{+x} + R_{U\text{B}}^{-x}, \tag{4}$$

where d_1 is a minimal distance between A and B atoms.

The main disadvantage of this approach is that in many cases the internuclear distances (A-B) in compounds and alloys are lower than the value of d_{min}.

Additional criteria are necessary to translate the system (2) – (4) into the language of quantum chemistry. It is necessary to take into account that the spherical symmetry of the electron density is broken in the zone of bonding localized orbitals and for $d_1 < d_{min}$ the formation of bonds (A-B) is accompanied by the transition of electrons to other directions of interatomic interaction, and this bond becomes donor. This condition is fulfilled if the extraction ($+\Delta e$) of electrons or their localization ($-\Delta e$) of the charges that a given pair has at a given direction of the bond equally change the values of the charges that a given pair has at $d_1 = d_{min}$, i.e. $Z_{\text{eфA(B)}} = Z_{min\text{A(B)}} + \left(\frac{\Delta e}{2}\right)$. These conditions are described by the system of equations:

$$lgR_{UA}^{ZA} = lgR_{UA}^{0} - (Z_{minA} + \tfrac{\Delta e}{2})tg\alpha_{\text{A}}, \tag{5}$$

$$lgR_{U\text{B}}^{ZB} = lgR_{U\text{B}}^{0} - (Z_{minB} + \tfrac{\Delta e}{2})tg\alpha_{B} \tag{6}$$

$$d_1 = R_{UA}^{ZA} + R_{U\text{B}}^{ZB}, \tag{7}$$

Equations (2) – (4) and (5) – (7) are similar, but replacing x with $(Z_{min} + \frac{\Delta e}{2})$ changes their physical meaning. The function $d_1 = f(Z_{\text{eф}})$ is calculated according to the crystal chemical approach ($Z_A = -Z_{\text{B}}$), is correct only for $d_1 = d_{min}$, but this is enough for the system (5) – (7) to be solved for a known d_1.

Considering the quantum interpretation of the empirical material enabled obtaining an expression for the energy of chemical bonds in the form:

$$D^{i}_{A-B} = \left(\frac{C_1(R^0_{UA}+R^0_{UB})}{(\mathrm{tg}\,\alpha_A+\mathrm{tg}\,\alpha_B)}\right)\left(\frac{C_2 d_i}{d_i^2-R_{UA}R_{UB}}-\frac{1}{d_i}\right), \tag{8}$$

where $R^0_{UA(B)}$, $tg\alpha_{\mathrm{A(B)}}$ are coefficients of equations (2) – (4) for atoms A and B; R_{UA} and R_{UB} are effective radii of their ions in bonds (A-B) of length d_i; i are the number of non-equivalent interatomic distances in the compounds and alloys under consideration; C_1 is a coefficient reflecting the relationship between the dimensional and energetic characteristics of interatomic interactions (measured in electron volts); C_2 is a coefficient, depending on the crystal structure and chemical bond and is chosen to be dimensionless.

Using the given equations, calculations of effective charges, effective radii and dissociation energies of chemical bonds of Bi-Sn-Te compounds and alloys were performed.

The results of calculations of R^0_U and $tg\alpha$ of the initial components are given in Table 1.

Table 1.

Coefficients $\mathrm{R}^0_{\mathrm{U}}$ and tgα of the initial components

Z	Element	R^0_U(Å)	$tg\alpha$
83	Bi	1.63	0.068
52	Te	1.57	0.076
50	Sn	1.35	0.0725

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ at various interatomic distances $d_i (1 \le i \le 9)$ of the structural modifications of Bi, Sn, BiTe are presented in tables (2) – (7).

In the given tables, the values of the coefficients C_1 and C_2 in the calculations in the first approximation are chosen equal to unity.

The properties of the material, determined by the gradient of any parameter, depend on the geometry of the structure. In the simplest case, this dependence is associated with various methods of energy transfer. In other cases, though, the behavior of each phase depends on the characteristics of adjacent phases. In this case, the method of finding the averaged characteristics will depend on the shape and distribution of each phase component. For example, the thermal conductivity and electrical conductivity of multiphase materials are subject to the rule of mixtures. Fig. 6 shows the dependence of thermal conductivity on the distribution of phases (structure models).

Models of this type can also be used for electrical conductivity. Fig. 6a shows the parallel distribution of phases f_i. In such a model, parallel conductivity occurs, therefore

$$k_{\text{м}} = f_1k_1 + f_2k_2 + \ldots, \tag{9}$$

where $k_{\text{м}}$ stands for the average thermal conductivity of the material.

Table 2.

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ depending on interatomic distances d_i Bi-Bi

NHO Bi-Bi	Bi-Bi								
.Parameters	φ1	φ2	φ3	φ4	φ5	φ6	φ7	φ8	φ9
d_i (Å)	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
$R^{Bi}_{U_i}$ (Å)	1.35	1.4	1.45	1.5	1.55	1.6	1.65	1.7	1.75
$\Delta q_i\ (\varphi_i)$	1.2037	0.9715	0.7473	0.531	0.321	0.12	-0.078	-0.269	-0.442
$D(\varphi_i)$ (eV)	2.96	2.854	2.755	2.663	2.578	2.497	2.421	2.35	2.35

Table 3.

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ depending on interatomic distances d_i Sn-Sn

NHO Sn-Sn	Sn-Sn								
Parameters	φ1	φ2	φ3	φ4	φ5	φ6	φ7	φ8	φ9
d_i (Å)	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
$R^{Bi}_{U_i}$ (Å)	1.35	1.4	1.45	1.5	1.55	1.6	1.65	1.7	1.75
$\Delta q_i\ (\varphi_i)$	0	-0.218	-0.428	-0.631	-0.828	-1.018	-1.202	-1.381	-1.554
$D(\varphi_i)$ (eV)	2.3	2.217	2.14	2.069	2.002	1.94	1.881	1.826	1.774

Table 4.

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ depending on interatomic distances d_i Te-Te

NHO Te-Te	Te-Te								
Parameters	φ1	φ2	φ3	φ4	φ5	φ6	φ7	φ8	φ9
d_i (Å)	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
$R^{Bi}_{U_i}$ (Å)	1.35	1.4	1.45	1.5	1.55	1.6	1.65	1.7	1.75
$\Delta q_i\ (\varphi_i)$	0.663	0.655	0.454	0.261	0.073	-0.108	-0.264	-0.455	-0.62
$D(\varphi_i)$ (eV)	2.551	2.46	2.755	2.295	2.221	2.152	2.087	2.025	1.968

Table 5.

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ depending on interatomic distances d_iBi-Te

NHO Bi-Te / Parameters	Bi-Te								
	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9
d_i (Å)	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
$R_{U_i}^{Bi}$ (Å)	1.350	1.438	1.48	1.535	1.58	1.63	1.68	1.728	1.77
$R_{U_i}^{Te}$ (Å)	1.31	1.362	1.42	1.465	1.52	1.57	1.62	1.672	1.73
Δq_i (φ_i)	1	0.8	0.6	0.4	0.2	0	-0.2	-0.36	-0.54
$D(\varphi_i)$ (eV)	2.74	2.643	2.552	2.467	3.388	2.314	2.262	2.178	2.116

Table 6.

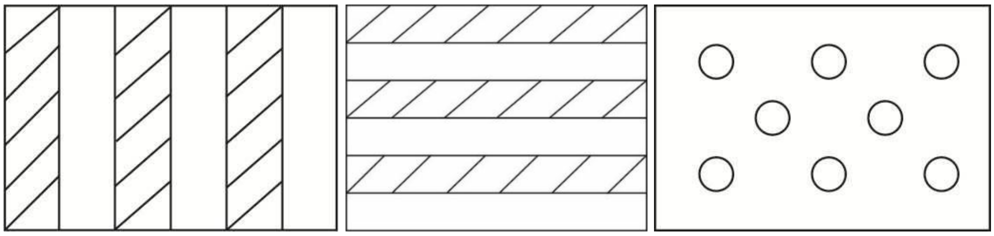
Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ depending on interatomic distances d_iBi-Sn

NHO Bi-Sn / Parameters	Bi-Sn								
	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9
d_i (Å)	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
$R_{U_i}^{Bi}$ (Å)	1.48	1.53	1.588	1.64	1.694	1.7465	1.8	1.853	1.905
$R_{U_i}^{Sn}$ (Å)	1.22	1.27	1.312	1.36	1.406	1.4535	1.5	1.547	1.595
Δq_i (φ_i)	0.58	0.4	0.1684	-0.0414	-0.2443	-0.4408	-0.631	-0.816	-0.9954
$D(\varphi_i)$ (eV)	2.586	2.4085	2.4085	2.329	2.2545	2.185	2.1	2.057	1.99923

Table 7.

Effective charges (Δq_i), effective radii (R_{Ui}) and dissociation energies $D(\varphi_i)$ depending on interatomic distances d_iSn-Te

NHO Sn-Te / Parameters	Sn-Te								
	φ_1	φ_2	φ_3	φ_4	φ_5	φ_6	φ_7	φ_8	φ_9
d_i (Å)	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5
$R_{U_i}^{Sn}$ (Å)	1.251	1.2957	1.341	1.386	1.431	1.475	1.52	1.565	1.61
$R_{U_i}^{Te}$ (Å)	1.449	1.5038	1.559	1.614	1.669	1.725	1.78	1.835	1.89
Δq_i (φ_i)	0.4584	0.246	0.040	-0.1583	-0.35	-0.5296	-0.716	-0.8908	-1.06
$D(\varphi_i)$ (eV)	2.4102	2.3237	2.243	2.168	2.098	2.032	1.97	1.912	1.857



a) b) c)

Fig. 6. Dependence of thermal conductivity on phase distribution (structure models).

In the case of model b) the representation of serial conductivity is applied and accordingly:

$$\frac{1}{k_M} = \frac{f_A}{k_A} + \frac{f_B}{k_B} + \ldots, \tag{10}$$

For the case of a two-phase structure, we will have:

$$k_M = \frac{k_A + k_B}{f_A k_A + f_B k_B}, \tag{11}$$

In case c) a matrix with a dispersed phase is depicted. Depending on the form of the phase, the modes of averaging may be different.

The results obtained in this work are in good agreement with the stages of creating anti-diffusion and connecting structures given in [4], which should have contact connections between n- and p-type legs compatible in terms of physicochemical properties; minimal losses at electrical and thermal junctions; high stability; sufficient mechanical strength; and resistance to thermal changes.

Conclusions

The results in tables (2) – (7) demonstrate that, with increasing interatomic distances, the dissociation energy of chemical bonds decreases, and the redistribution of electron density changes sign in a wide range of interatomic distances:

Bi-Bi ($3{,}2 \le d_1 \le 3{,}3$); Bi-Te ($3{,}2 \le d_1 \le 3{,}3$);
Te-Te ($3{,}1 \le d_2 \le 3{,}2$); Bi-Sn ($2{,}9 \le d_3 \le 3$);
Sn-Te ($2{,}9 \le d_3 \le 3$); Sn-Sn ($2{,}7 \le d_4 \le 2{,}8$);

This means that chemical bonds can be both “donors” and "acceptors" under certain conditions, i.e., they can both improve and worsen the quality of the Bi-Sn-Te based thermoelectric material and the quality of connection.

Thus, the use of the obtained results of studies of the electronic properties of Bi, Sn, Te Bi-Te, Bi-Sn, Sn-Te enables predicting the form of the liquidus, and hence the type of melting of the resulting Bi-Sn-Te based material.

The results of calculations of effective charges, dissociation energies, and effective radii obtained in the work are in good agreement with the results of thermal rearrangement of atoms during the formation of short-range order of chemical bonds and expand technological possibilities when considering phase transformations caused by the destruction of existing bonds and the formation of new ones.

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Теоретичні моделі впорядковуваних сплавів термоелектричних матеріалів на основі Bi-Sn-Te

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Розроблено комплексний підхід для побудови теоретичних моделей упорядкованих сплавів на основі Bi-Sn-Te. Представлено розрахунки ефективних радіусів, перерозподілу електронної густини та енергії дисоціації нееквівалентних гібридних орбіталей (НГО) в системі Bi-Sn-Te в залежності від міжатомних віддалей. Запропоновано схему вдосконалення технології комутації гілок термоелемента з урахуванням особливостей хімічного зв'язку.

Ключові слова: теоретичні моделі, хімічний зв'язок, ефективні радіуси, електронна густина, діаграми стану.