UDC 544.344.015.3: 546.81'86'23

MULTI-3D MODELING OF PHASE DIAGRAM OF $PbTe$-Bi_2Te_3-Sb_2Te_3 SYSTEM

A.I. Aghazade[1], S.M. Rustamova[3], I.M. Gojayeva[1], E.N. Orujlu[2], D.M. Babanly[1.2], A.N. Mammadov[1,3]

[1] Institute of Catalysis and Inorganic Chemistry of MSE Azerbaijan Republic, AZ 1143, H. Javid Ave. 113, Baku, Azerbaijan
[2] Azerbaijan State Oil and Industry University, French - Azerbaijani University, AZ 1010, Azadlyg Ave. 20, Baku, Azerbaijan
[3]Azerbaijan Technical University, AZ1073, H. Javid Ave. 25, Baku, Azerbaijan
e-mail: aytenagazade94@gmail.com

Received 12.07.2023
Accepted 04.09.2023

Abstract. *Using the analytical option of the Origin Lab computer program, the analytical dependences of the liquidus temperature on the composition for the $PbTe$-Bi_2Te_3, $PbTe$-Sb_2Te_3, Bi_2Te_3-Sb_2Te_3 boundary systems of the $PbTe$-Bi_2Te_3-Sb_2Te_3 ternary system were determined. Based on these dependencies and thermal analysis data of the ternary system, the analytical model of the temperature-composite dependence of the crystallization surfaces of $PbTe$, Sb_2Te_3, Bi_2Te_3 compounds and $PbBi_2Te_4$, $PbBi_4Te_7$, $PbBi_6Te_{10}$ phases in the $PbTe$-Bi_2Te_3-Sb_2Te_3 system was determined. The resulting equations made it possible to visualize the phase diagram of the $PbTe$-Bi_2Te_3-Sb_2Te_3 system from the side of the $PbTe$-Bi_2Te_3 in 3D coordinates. The analytical model of the phase diagram of the $PbTe$-Bi_2Te_3-Sb_2Te_3 system allowed constructing a three-dimensional image of equilibrium phases from different angles, to obtain two-dimensional projections and to tabulate the coordinates of the phase diagram.*

Keywords: *$PbTe$-Bi_2Te_3-Sb_2Te_3 system, 3D analytical modeling, phase diagram, liquidus, solidus.*
DOI: 10.32737/2221-8688-2023-4-353-360

1. Introduction

One of the main problems of materials science is the design of new functional materials and the expansion of their existence horizons by optimizing the desired properties and new prospects for application in various fields. In recent years, a lot of theoretical and experimental work has been done to create the thermoelectric materials, which are considered as main method to solve the problems of fuel use and energy harvesting [1-3]. Lead tellurides-based alloys are the most successfully applied thermoelectric materials used in the production of similar materials [4,5]. Also, tetradymite-type layered Bi_2Te_3-based alloys are classic low-temperature thermoelectric materials, and recently, their electrical and thermal properties have been enhanced through nanostructuring [6,7].

As the information on topological insulators increased [8, 9], layered bismuth and antimony chalcogenides were also proven to host topological surface states [10-12]. Ongoing research in this field revealed that tetradymite-like ternary compounds formed in A^{IV} –B^{V} –Te systems (A^{IV}–Ge, Sn, Pb; B^{V}–Sb, Bi) systems including $A^{IV}B^{V}_2Te_4$, $A^{IV}B^{V}_4Te_7$, $A^{IV}B^{V}_6Te_{10}$ are also three-dimensional topological insulators [13-21]. The creation of new multicomponent functional materials is possible based on the phase equilibria data of the corresponding systems. The desired properties can be achieved by substituting appropriate elements in these materials via the formation of solid solutions [22-25].

The main principle of building a three-dimensional (3D) computer model of a T-x-y diagram of a ternary system is the construction of three-dimensional images of its surfaces and

phase regions. It may take a lot of time and additional experiments to create the ideal model. However, the computer model does not contain the methodological errors detected during the construction of phase diagrams using traditional methods [26].

The phase relationship in the PbTe-Bi_2Te_3-Sb_2Te_3 system was studied by using powder XRD, DTA, and SEM results of the equilibrated alloys [27,28]. In this research, the analytical method was used for 3D modeling of crystallization surfaces of the PbTe-Bi_2Te_3-Sb_2Te_3 system based on the data of boundary systems and a small number of experimental DTA measurements.

2. Modeling Technique

The analytical method, tested in [29-31], was used for the three-dimensional modeling of crystallization surfaces in the PbTe-Bi_2Te_3-Sb_2Te_3 system. For 3D modeling of crystallization surfaces of phases the following equation was used:

$$T_{1(1-2-3)}=yT_{1(1-2)}(x_1)+(1-y)T_{1(1-3)}(x_1)+ax_1(1-x_1)^2y(1-y) \quad (1)$$

Here $y=x_2/(x_2+x_3)$, $y=x_3/(x_2+x_3)$, x_1, x_2 and x_3– are mole fraction of 1, 2, 3 components; $T_{1(1-2)}$ and $T_{1(1-3)}$ – are liquidus temperatures for boundary binary systems 1-2 and 1-3. The parameter a_1 is determined from the experimental data of the ternary system PbTe-Bi_2Te_3-Sb_2Te_3.

Modeling is made in the following order. First, the temperature dependences on the composition $T = f(x)$ and $T = f(y)$ were determined for the liquidus of boundary binary systems. Next, based on the experimental data of the PbTe-Bi_2Te_3-Sb_2Te_3 ternary system, the function $T = f(x,y)$ is defined, where: x-=x(PbTe): y=x(Bi_2Te_3)/[x(Sb_2Te_3)+ x(Bi_2Te_3)]; x_i – molar fractions of PbTe, Bi_2Te_3, Sb_2Te_3 compounds. To determine the boundaries of immiscibility of liquid alloys, the asymmetric version of the model of regular solutions

$$\Delta G_T^0 = [a + b(1-x)^2](1-x)x + RT[xlnx(1-x)\ln(1-x)] \quad (2)$$

And the thermodynamic condition for internal stability

$$(\partial^2\Delta G^0/\partial x^2)_{P,T}=-2*(a+b*x\text{^}2+2*b*x*(x-1)+b*x*(3*x-1))+8.31*T/(1-x)+8.31*T/x \quad (3)$$

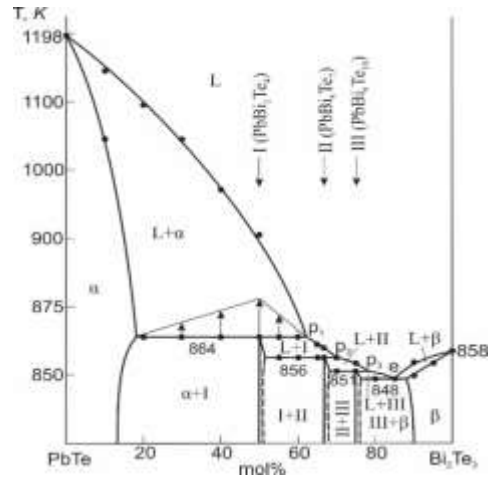
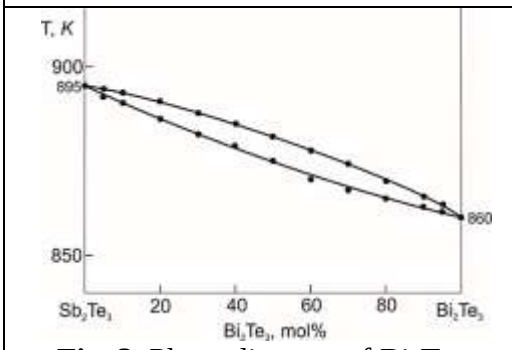
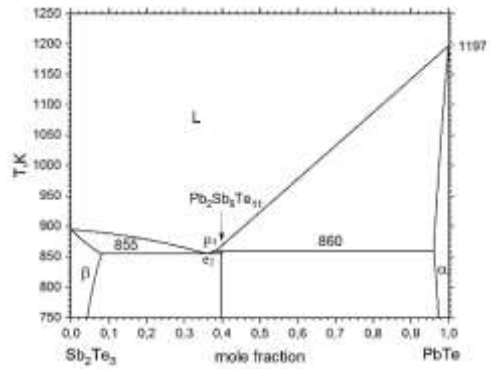
were used. The obtained analytical expressions for the PbTe-Bi_2Te_3-Sb_2Te_3 ternary system and its boundary binary systems are given in Tables 1 and 2. The analytical dependencies are given in the form used by the Origin Lab computer program.

2.1. Boundary binary systems

The boundary sides of the analyzed system were studied. According to PXRD (Powder X-ray Diffraction) and DTA (Differential Thermal Analysis) data, the existence of three $PbBi_2Te_4$, $PbBi_4Te_7$, and $PbBi_6Te_{10}$ tetradymite-like layered ternary compounds was confirmed. All listed ternary compounds melt by peritectic reactions at 864, 856, and 851 K, respectively [32]. According to [33-35], two members of $nPbTe{\cdot}mSb_2Te_3$ homologues series, namely, $PbSb_2Te_4$ and $PbSb_4Te_7$ are formed in the PbTe-Sb_2Te_3 system, while further studies [35-39] show that earlier reported $Pb_2Sb_6Te_{11}$ compound is stable only in a small temperature range and decomposes by solid-phase reaction. The Bi_2Te_3-Sb_2Te_3 system is characterized by the formation of continuous solid solutions with a tetradymite-like structure [21].

Here and throughout the text, the following notation is adopted: α-is solid solutions based on PbTe; β-is solid solutions based on Bi_2Te_3 and Sb_2Te_3.

Table 1. Phase diagrams and analytical dependencies for liquidus and solidus surfaces of the PbTe-Bi_2Te_3, PbTe-Sb_2Te_3, and Sb_2Te_3–Bi_2Te_3 systems (equations are presented in computer variation).

Phase diagrams	System, region x=x(Bi_2Te_3)	Equations: T,K=f(x) x=x(Bi_2Te_3)	Eq. N.
 **Fig. 1.** Phase diagram of PbTe-Bi_2Te_3 [32] system	Bi_2Te_3-PbTe. liquidus α-PbTe, x= 0÷0.62	1198-288.4*x-1224*x^2+1321*x^3	4
	liquidus p_1p_2, x=0.62÷0.7	694.5+593.7*x-518.5*x^2	5
	liquidus p_2p_3e, x=0.7÷0.825	776.4+264,5*x-215.4*x^2	6
	liquidus β-Bi_2Te_3, x=0.85÷1	654+354*x-148*x^2	7
	solidus α-PbTe, x=0÷0.18	1198-238*x-20458*x^2+63470*x^3	8
	solidus α-PbTe, x=0.12÷0.18	473+4510*x-13000*x^2	9
	solidus β-Bi_2Te_3, x=0.88÷1	760+100*x	10
	solidus β-Bi_2Te_3, x=0.88÷0.91	-9155+23100*x-13333*x^2	11
 **Fig. 2.** Phase diagram of Bi_2Te_3-Sb_2Te_3 [20] system	Bi_2Te_3- Sb_2Te_3. x=x(Bi_2Te_3)=0÷1 liquidus	895-35*x+15*x*(1-x)	12
	x=x(Bi_2Te_3)=0÷1 solidus	895-35*x-15*x*(1-x)	13
 **Fig. 3.** Phase diagram of Sb_2Te_3-PbTe [39] system	Sb_2Te_3-PbTe liquidus α-PbTe x=x(PbTe)=0.38÷1	653+539*x+5.8*x^2	14
	liquidus p_4e_2, x= x(PbTe)=0.36÷0.38	765+250*x	15
	liquidus β-Sb_2Te_3 x=x(PbTe)=0÷0.36	895-46*x-180*x^2	16
	solidus β-Sb_2Te_3 x=x(PbTe)=0÷0.08	895-650*x+1875*x^2	17
	solidus β-Sb_2Te_3 x=x(PbTe)=0.05÷0.1	555+5750*x-25000*x^2	18
	solidus α-PbTe x=x(PbTe)=0.96÷1	58828+113775*x-53750*x^2	19
	solidus α-PbTe x=x(PbTe)= 0.96÷0.94	446+4325*(1-x)-10545*(1-x)^2	20

2.2.System $PbTe-Bi_2Te_3-Sb_2Te_3$

Analytical dependencies of the 3D modeling of the phases of the $PbTe-Bi_2Te_3-Sb_2Te_3$ system are given in Table 2 (equations 21-28).

Table 2. Analytical dependencies of the phases of the $PbTe-Bi_2Te_3-Sb_2Te_3$ system.

Phase number in Fig. 4.	T,K=f(x,y); x=x(PbTe): y= $x(Bi_2Te_3)/[x(Sb_2Te_3)+x(Bi_2Te_3)]$; x_i-mole fractions of the PbTe, Bi_2Te_3, Sb_2Te_3	Eq.N.
1	(1197-351*(1-x)-276.7*(1-x)^2-26.8*(1-x)^3)*y+ (653+539*x+5.8*x^2)*(1-y)+70*y*(1-y)*(1-x) x=0÷0.625, y=0÷1	21
2	(1197-1465,3*x+9728*x^2-91304*x^3)*(1-y)+(1079-1923,1*x+5841,7*x^2-6624,48*x^3)*y-48*y*(1-y), x=0.842÷1, y=0÷1; (446+4325*x-10545*x^2)*(1-y)+ (443,5+2065*x)*y, x=0.954÷0.832, y=0÷1	22
5	694.5+593.7*(1-x)-518.5*(1-x)^2)*y+(765+250*x)*(1-y) +70*y*(1-y)*(1-x) x=0.625÷0.71, y=0÷0.95	23
6	(776,4+264,5*x-215,4*x^2)*(1-y)+(596,6+677,5*x-437,5*x^2)*y, x=0.695÷0.875, y=0÷1	24
7	(546+592*x-280*x^2)*(1-y)+(731+130*x)*y, x=0.81÷0.875, y=0÷1	25
9	(629,6+421,9*(1-x)-190,5*(1-x)^2)*y+(895-46*x-180*x^2)*(1-y)+ 70*y*(1-y)*(1-x); y=0÷1	26
11	(-13642+34100*x-20000*x^2). x=0.9÷0.97, y=0÷1	27
12,13,14	12550+26300*x; 9542-26300*x; -5975+26300*x	28

According to the numbers of the indicated fragments of the phase diagram of the $PbTe-Bi_2Te_3-Sb_2Te_3$ system, T,K=f(x,y) are visualized in Fig 4:

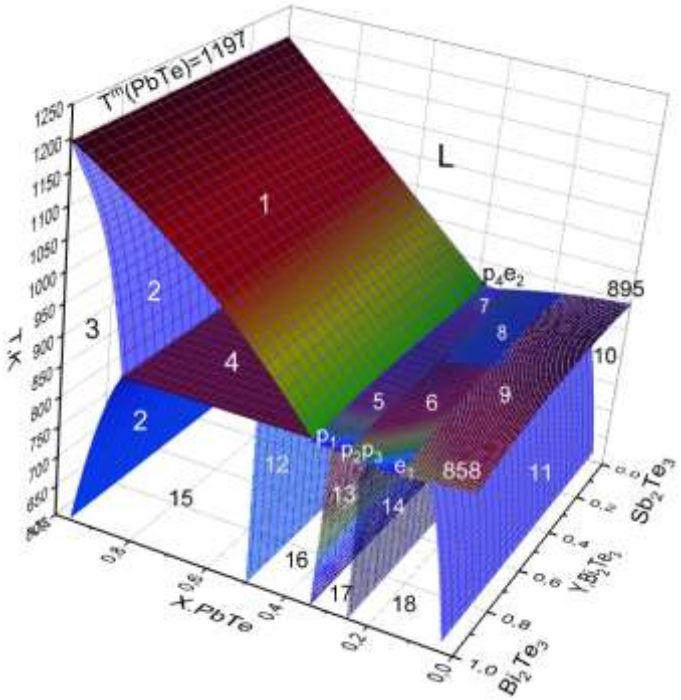


Fig. 4. 3D view of the phase diagram of the $PbTe-Bi_2Te_3-Sb_2Te_3$ system from the side of the $PbTe-Bi_2Te_3$ system.

1- Liquid surface of solid solutions based on α-PbTe;
2- Solidus surface of solid solutions based on α-PbTe;
3- Solid solution based on α-PbTe;
4- Plane obtaining peritectic $PbBi_2Te_4$ compound
5- Liquidus surface of the peritectic $PbBi_2Te_4$ compound;
6- Liquidus surface of peritectic $PbBi_4Te_7$ and $PbBi_6Te_{10}$ compounds;
7- Liquidus surface of the peritectic $Pb_2Bi_6Te_{11}$ compound;
8- Liquid surface of solid solutions based on β-Bi_2Te_3;
9- Liquid surface of solid solutions based on β-Bi_2Te_3 and β-Sb_2Te_3;
10- Solid solution based on β-Bi_2Te_3 and β-Sb_2Te_3;
11- Solidus surface of solid solutions based on β-Bi_2Te_3 and β-Sb_2Te_3;
12-14- Planes perpendicular to obtaining peritectic phases $PbBi_2Te_4$, $PbBi_4Te_7$, $PbBi_6Te_{10}$;
15- Heterogeneity areas of solid solutions based on α-PbTe-+ $PbBi_2Te_4$;
16- Heterogeneity area of $PbBi_2Te_4$ + $PbBi_4Te_7$ phase;
17- Heterogeneity area of $PbBi_4Te_7$ + $PbBi_6Te_{10}$ phase;
18- Heterogeneity area of $PbBi_6Te_{10}$+ solid solutions based on β-Bi_2Te_3 and β-Sb_2Te_3.

3. Conclusion

The use of 3D modeling made it possible to determine the analytical dependences of integral and partial thermodynamic properties depending on the mole fractions of all components in the entire concentration range (x_i=0÷1) in the 300-1250 K temperature range.

Based on obtained data, the homogeneity areas of stable solid solutions and the areas of the formation of ternary compounds and the multiphase diagram of the PbTe-Sb_2Te_3-Bi_2Te_3 system in three-dimensional space were determined. Analytical dependences, in the form of 3D model, according to the analytical option of the Origin Lab program, contain, respectively, 100x100 = 10,000 and 50x50 = 2500 tabular data in the form of matrices that can be used for choose the optimal values of the composition, and temperature for the synthesis of PbTe, Bi_2Te_3, Sb_2Te_3 binary compounds and three-component phases in the PbTe-Bi_2Te_3 - Sb_2Te_3 system.

The obtained 3D model of the phase diagram also makes it possible to better understand the crystallization processes in the system via visualization of liquidus and solidus surfaces.

Acknowledgment
The work was supported by the Azerbaijan Science Foundation - **Grant № AEF-MCG-2022-1(42)-12/10/4-M-10.**

References

1. Morelli D.T. Thermoelectric Materials. In: Kasap S., Capper P. (eds) Springer Handbook of Electronic and Photonic Materials. Springer Handbooks. Springer, Cham. 2017, pp. 1379-1390.
2. Shevelkov A.V. Chemical aspects of the design of thermoelectric materials. *Russian Chemical Reviews*, 2008, vol. 77, no. 1, pp. 1-19.
3. Gayner C., Kar K.K. Recent advances in thermoelectric materials. *Progress in Materials Science*, 2016. vol. 83. pp. 330–382.
4. LaLonde A.D., Pei Y., Wang H., Snyder G.J. Lead telluride alloy thermoelectrics. /*Materials Today*, 2011, vol. 14, no. 11, pp. 526-532.
5. Fu L., Yin M., Wu D., Li W., Feng D., Huang L., He J. Large enhancement of thermoelectric properties in n-type PbTe via dual-site point defects. *Energy & Environmental Science*, 2017, vol. 10, pp. 2030-2040.
6. Hong M., Chen Z. G., Zou J. Fundamental and progress of Bi_2Te_3-based

thermoelectric materials. *Chinese Physics B*, 2018, vol. 27, p. 048403.
7. Poudel B., Hao Q., Ma Y., Lan Y., Minnich A., Yu B., Yan X., Wang D., Muto A., Vashaee D., Chen X., Liu J., Dresselhaus M.S., Chen G., Ren Z. High-thermoelectric performance of nanostructured bismuth antimony telluride bulk alloys. *Science*, 2008, vol. 320, pp. 634-638.
8. Qi X.L., Zhang S.C. Topological insulators and superconductors. *Reviews of Modern Physics*, 2011, vol. 83, pp. 1057.
9. Qi X.L., Zhang S.C. The quantum spin Hall effect and topological insulators. *Physics Today*, 2010, vol. 63, no. 1, p. 33.
10. Hu L., Gao H., Liu X., Xie H., Shen J., Zhu T., Zhaoa X. Enhancement in thermoelectric performance of bismuth telluride based alloys by multi-scale microstructural effects, *Journal of Materials Chemistry*, 2012, no. 22, p. 16484.
11. Lamuta, C., Campi D., Cupolillo A., Aliev Z.S., Babanly M.B., Chulkov E.V., Politano A., Pagnotta L. Mechanical properties of Bi_2Te_3 topological insulator investigated by density functional theory and nanoindentation. *Scripta Materialia*, 2016, vol. 121, pp. 50–55.
12. Heremans J.P., Cava R.J., Samarth N. Tetradymites as thermoelectrics and topological insulators. *Nature Reviews Materials*, 2017, no. 2, pp. 17049.
13. Zhang H., Liu C.X., Qi X.L., Dai X., Fang Z., Zhang S.C. Topological insulators in Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3 with a single Dirac cone on the surface. *Nature Physics*, 2009, vol. 5, no.6, pp. 438–442.
14. Flammini R., Colonna S., Hogan C., Mahatha S., Papagno M., Barla A., Sheverdyaeva P., Moras P., Aliev Z., Babanly M.B. Evidence of β-antimonene at the Sb/Bi_2Se_3 interface. *Nanotechnology*, 2018, vol. 29, no. 6, pp. 065704.
15. Politano A., Caputo M., Nappini S., Bondino F., Aliev Z.S., Babanly M.B., Chulkov E. Exploring the surface chemical reactivity of single crystals of binary and ternary bismuth chalcogenides. *Journal of Physical Chemistry C*, 2014, vol.118, pp.21517-21522.
16. Nurmamat M., Okamoto K., Zhu S., Menshchikova T.V., Rusinov I.P., Korostelev V.O., Miyamoto K., Okuda T., Miyashita T., Wang X., Ishida Y., Sumida K., Schwier E.F., Ye M., Aliev Z.S., Babanly M.B., Amiraslanov I.R., Chulkov E.V., Kokh K.A., Tereshchenko O., Shimada K., Shin S., Kimura A. Topologically non-trivial phase-change compound $GeSb_2Te_4$. *ACS Nano*, 2020, vol. 14, no. 7, pp. 9059–9065.
17. Pacilè D., Eremeev S.V., Caputo M., Pisarra M., De Luca O., Grimaldi I., Fujii J., Aliev Z.S., Babanly M.B., Vobornik I., Agostino R.G., Goldoni A., Chulkov E.V., Papagno M. Deep Insight Into the Electronic Structure of Ternary Topological Insulators: A Comparative Study of $PbBi_4Te_7$ and $PbBi_6Te_{10}$. *physica status solidi (RRL) – Rapid Research Letters*, 2018, vol. 12, no.12, p. 1800341.
18. Shvets I.A., Klimovskikh I.I., Aliev Z.S., Babanly M.B., Sánchez-Barriga J., Krivenkov M., Shikin A.M., Chulkov E.V. Impact of stoichiometry and disorder on the electronic structure of the $PbBi_2Te_{4-x}Se_x$ topological insulator. *Physical Review B*, 2017, vol. 96, pp. 235124 -7.
19. Li R., Liu G., Jing Q., Wang X., Wang H., Zhang J., Ma Y. Pressure-induced superconductivity and structural transitions in topological insulator $SnBi_2Te_4$. *Journal of Alloys and Compounds*, 2022, vol. 900, p.163371.
20. Orujlu E.N., A.E. Seidzade A.E., Aliev Z.E., Amiraslanov I.R.,Babanly M.B. Synthesis and crystal structure of a new 9P–Type layered Van der Waals compound $SnBi_4Te_4$. *Chemical problems*. 2020, vol. 18, no. 1, pp. 40-48.
21. Babanly M.B., Chulkov E.V., Aliev Z.S., Shevelkov A.V., Amiraslanov I.R. Phase diagrams in materials science of topological insulators based on metal chalcogenides. *Russian Journal of Inorganic Chemistry*, 2017, vol. 62, pp. 1703-1729.
22. Mammadov A.N., Asadov M.M., Mustafaeva S.N., Tagiev D.B.. Effect of Composition on the Physical Properties of $(TlInSe_2)_{1-x}(TlGaTe_2)_x$ Solid Solutions. *Inorganic Materials*, 2015, vol.51, no.12, pp.1232-1236.

23. Orujlu E.N. Phase relations and characterization of solid solutions in the $SnSb_2Te_4$-$MnSb_2Te_4$ system. *New Materials, Compounds and Applications*, 2020, vol. 4, no. 1, pp. 38-43.
24. Orujlu E.N., Ziya S.A., Babanly M.B. The phase diagram of the MnTe–SnTe–Sb_2Te_3 ternary system and synthesis of the iso-and aliovalent cation-substituted solid solutions. *Calphad*, 2022, vol. 76, pp. 102398.
25. Hattori Y., Tokumoto Y., Kimoto K., Edagawa K. Evidences of inner Se ordering in topological insulator $PbBi_2Te_4$-$PbBi_2Se_4$-$PbSb_2Se_4$ solid solutions. *Scientific Reports*, 2020, vol. 10, pp. 7957.
26. Mamedov A.N., Salimov Z.E., Mashadiyeva L.F., Babanly M.B. Thermodynamic calculation and 3D modeling of the liquidus and immiscibility surfaces of the Ge–Cu–Tl system. *American Chemical Science Journal*, 2016, vol. 10, no. 2, pp. 1-5.
27. Aghazade A.I., Orujlu E.N., Imamaliyeva S.Z., Mamedov A.N., Babanly M.B. New topological insulator phases of variable compositions in the PbTe-Sb_2Te_3 -Bi_2Te_3 system. Properties and Uses of Antimony – Editor: David J. Jenkins, Nova Science Publishers, 2022, pp. 95-112.
28. Aghazade A.I. Phase equilibria of the $PbBi_2Te_4$-"$PbSb_2Te_4$" section of the PbTe-Bi_2Te_3-Sb_2Te_3 system and some properties of the solid solutions. *Azerbaijan Chemical Journal*, 2020, no. 4, pp. 53-59.
29. Yusibov Yu.A., Alverdiev I.Dzh., Mashadieva L.F., Babanly D.M., Mamedov A.N., Babanly M.B. Experimental study and 3D modeling of the phase diagram of the Ag–Sn–Se system. *Russian Journal of Inorganic Chemistry*, 2021, vol. 63, no.12, pp. 1622-1635.
30. Ahmadov E.J., Mammadov A.N., Guliyeva S.A., Babanly M.B. Modeling of phase diagram of the system BiI_3-Bi_2S_3-Bi_2Te_3. *New Materials, Compounds and Applications*, 2021, vol. 5, no. 1, pp.5-11.
31. Hasanova G.S., Dashdiyeva G.B., Yusibov Y.A., Babanly M.B. Thermodynamic properties of the Bi_2Te_3 and Bi_4Te_5 compounds. *Chemical problems*, 2020, vol.18, no. 3, pp. 315-324.
32. Gojayeva I.M., Babanly V.I., Aghazade A.I., Orujlu E.N. Experimental reinvestigation of the PbTe–Bi_2Te_3 pseudo-binary system. *Azerbaijan Chemical Journal*, 2022, no. 2, pp. 47-53.
33. Karpinskii O.G., Shelimova L.E., Avilov E.S., Kretova M.A. X-ray Diffraction study of mixed-layer compounds in the PbTe-Bi_2Te_3 system. *Inorganic Materials*, 2002, vol. 38, no. 1, pp.17–24.
34. Shelimova L.E., Karpinskii O.G., Konstantinov P.P., Avilov E.S., Kretova M.A., Zemskov V.S. Crystal structures and thermoelectric properties of layered compounds in the ATe–Bi_2Te_3 (A = Ge, Sn, Pb) systems. *Inorganic Materials*, 2004, vol. 40, no. 5, pp. 451-460.
35. Shelimova L.E., Karpinskii O.G., Svechnikova T.E., Avilov E.S., Kretova M.A., Zemskov V.S. Synthesis and structure of layered compounds in the PbTe-Bi_2Te_3 and PbTe-Sb_2Te_3 systems. *Inorganic Materials*, 2004, vol. 40, no. 12, pp. 1264-1270.
36. Ikeda T., Collins L.A., Ravi V.A., Gascoin F.S., Haile S.M., Snyder G.J. Self-assembled nanometer lamellae of thermoelectric PbTe and Sb_2Te_3 with epitaxy-like interfaces. *Chemistry of Materials*, 2007, vol. 19, pp. 763-767.
37. Ikeda T., Haile S.M., Ravi V.A., Azizgolshani H., Gascoin F., Snyder G.J. Solidification processing of alloys in the pseudo-binary PbTe-Sb_2Te_3 system. *Acta Materiala*, 2007, vol. 55, no.4, pp.1227-1239.
38. Ikeda T., Toberer E.S., Ravi V.A., Snyder G.J., Aoyagi S., Nishibori E. In situ observation of eutectoid reaction forming a PbTe-Sb_2Te_3 thermoelectric nanocomposite by synchrotron X-ray diffraction. *Scripta Materialia*, 2009, vol. 60, no. 5, pp. 321-324.
39. Ikeda T., Snyder G.J. Nanostructure formation in bulk thermoelectric compounds in the pseudo binary PbTe-Sb_2Te_3 system. *Materials Research Society*, 2010, vol. 1267, pp. 1267- DD06-07.

МУЛЬТИ-3D МОДЕЛИРОВАНИЕ ФАЗОВОЙ ДИАГРАММЫ СИСТЕМЫ $PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$

А.И. Агазаде[1], С.М. Рустамова[3], И.М. Годжаева[1], Э.Н. Оруджлу[2], Д.М. Бабанлы[1,2], А.Н. Мамедов[1,3]

[1] Институт Катализа и Неорганической Химии,
Пр. Г.Джавида, 113, AZ 1143 Баку, Азербайджан
[2]Азербайджанский Государственный Университет Нефти и Промышленности,
Французско-Азербайджанский Университет
Пр. Азадлыг, 20, AZ 1010 Баку, Азербайджан
[3]Азербайджанский Технический Университет,
Пр. Г.Джавида, 25, AZ 1073 Баку, Азербайджан

Аннотация: С помощью аналитической опции компьютерной программы OriginLab определены аналитические зависимости температуры ликвидуса от состава для граничных систем $PbTe\text{-}Bi_2Te_3$, $PbTe\text{-}Sb_2Te_3$, $Bi_2Te_3\text{-}Sb_2Te_3$ тройной системы $PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$. На основании этих зависимостей и данных термического анализа тройной системы построена аналитическая модель поверхностей кристаллизации соединений PbTe, Sb_2Te_3, Bi_2Te_3 и фаз $PbBi_2Te_4$, $PbBi_4Te_7$, $PbBi_6Te_{10}$ в системе $PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$. Полученные уравнения позволили визуализировать фазовую диаграмму системы $PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$ со стороны $PbTe\text{-}Bi_2Te_3$ в трехмерных координатах. Аналитическая модель фазовой диаграммы системы $PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$ позволяет представить трехмерное изображение равновесных фаз с разных ракурсов, получить двумерные проекции и табулировать координаты фазовой диаграммы.

Ключевые слова: система $PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$, трехмерное аналитическое моделирование, фазовая диаграмма, ликвидус, солидус.

$PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$ SİSTEMİNİN FAZA DİAQRAMININ MULTİ-3D MODELLƏŞMƏSİ

A.İ. Ağazadə[1], S.M. Rüstəmova[1], İ.M. Qocayeva[1], E.N. Oruclu[2], D.M. Babanlı[1,2], A.N. Məmmədov[1,3]

[1] Kataliz və Qeyri-üzvi Kimya İnstitutu,
H.Cavid pr., 113, AZ 1143 Bakı, Azərbaycan
[2]Azərbaycan Dövlət Neft və Sənaye Universiteti,
Azərbaycan-Fransız Universiteti,
Azadlıq pr., 20, AZ 1010 Bakı, Azərbaycan
[3]Azərbaycan Texniki Universiteti,
H.Cavid pr., 25, AZ 1073 Bakı, Azərbaycan

Xülasə: OriginLab kompüter proqramının analitik variantından istifadə etməklə $PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$ üçlü sisteminin $PbTe\text{-}Bi_2Te_3$, $PbTe\text{-}Sb_2Te_3$, $Bi_2Te_3\text{-}Sb_2Te_3$ sərhəd sistemləri üçün likvidus temperaturunun tərkibdən analitik asılılıqları müəyyən edilmişdir. Bu asılılıqlar və üçlü sistemin termiki analizi məlumatları əsasında $PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$ sistemində PbTe, Sb_2Te_3, Bi_2Te_3 birləşmələrinin və $PbBi_2Te_4$, $PbBi_4Te_7$, $PbBi_6Te_{10}$ fazalarının kristallaşma səthlərinin analitik modeli işlənmişdir. Alınan tənliklər $PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$ sisteminin faza diaqramının $PbTe\text{-}Bi_2Te_3$ tərəfdən müxtəlif bucaqlardan üçölçülü təsvirini qurmağa, ikiölçülü proyeksiyalarını əldə etməyə və faza diaqramının koordinatlarını cədvəlləşdirməyə imkan verir.

Açar sözlər: $PbTe\text{-}Bi_2Te_3\text{-}Sb_2Te_3$ sistemi, 3D modelləşdirmə, faza diaqramı, likvidus, solidus.