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Ag–Sn–Se SYSTEM: PHASE DIAGRAM, THERMODYNAMICS AND MODELING**F.S.Ibrahimova***M.Nagiyev Institute of Catalysis and Inorganic Chemistry, NAS of Azerbaijan**ifs@live.ru*

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A comparative analysis of works on the study of phase equilibria, structures and thermodynamic properties of intermediate phases of the Ag–Sn–Se ternary system has been carried out. It was shown that two ternary compounds Ag_8SnSe_6 and AgSnSe_2 are formed in the system, melting congruently at 1015 K and incongruently at 860 K, respectively. The most reliable data for enthalpy, entropy, free formation energy, and heat capacities of AgSnSe_2 and the argirodit phase of Ag_8SnSe_6 are recommended. Thermodynamic functions of mixing liquid solutions are approximated by an asymmetric version of the model of regular solutions. To determine the boundaries of the separation of liquid alloys, the function of the internal thermodynamic stability of the homogeneous phase was used. With the help of the program OriginLab, multi 3D visualization of Ag_2Se , SnSe_2 , SnSe , Ag_8SnSe_6 crystallization surfaces and immiscibility surfaces in the Ag–Sn–Se system was carried out.

Keywords: copper–lead–tellurium system, phase diagram, the surface of the liquidus, 3D modeling.

doi**Introduction**

The growing interest to the Ag–Sn–Se system is due to the fact that silver-tin selenides, in particular the Ag_8SnSe_6 compound, and other representatives of natural minerals Argyrodites have mixed ionic-electronic conductivity in combination with high thermoelectric and optical properties, superconductivity [1–3]. Therefore, silver-tin selenides are promising materials for use in photo-electrodes, electrochemical converters of solar energy, ion-selective sensors, photoelectrochemical visualizations [4–8]. The phase equilibria in the Ag–Sn–Se system have been investigated in a number of papers [9–15]. However, the results of these studies on phase equilibria and thermodynamic parameters are often different. In recent years, work has appeared on 3D modeling of mono- and non-invariant equilibria in this system. The purpose of this review is to analyze and systematize the works on the study of phase diagrams, structures and thermodynamic properties of intermediate phases of the Ag–Sn–Se ternary system.

Phase diagram and properties of ternary compounds

The phase diagrams of this system were first studied in [9] with the construction of the Ag_2Se – SnSe_2 quasi-binary cross section state diagram. It was shown that a single ternary compound Ag_8SnSe_6 with incongruent melting

at 1008 K and a polymorphic transition at 356 K is formed in this section. However, in [10], the Ag_2Se – SnSe_2 cut is not quasibinary, and the Ag_8SnSe_6 compound melts congruently at 1027 K a later published paper [11] reported on the synthesis of a compound Ag_2SnSe_3 . The Ag_2Se – SnSe cross section was studied in [12–15]. According to [12, 14, 15], this section is quasi-binary and belongs to the eutectic type: the crystallization temperatures of the eutectic are 824, 818 and 883 K, respectively. In [13], it is reported that the Ag_2Se – SnSe cut is not quasibinary due to the presence of a field of primary crystallization of free silver. A complete diagram of the Ag–Sn–Se system is presented in [10] with the determination of the liquidus surface, on which the ternary compounds Ag_8SnSe_6 and AgSnSe_2 and two immiscibility areas are reflected. In [13], the phase equilibrium picture in the region of Ag– Ag_2Se – Ag_8SnSe_6 – SnSe –Sn composition is slightly different from [10]. In [13], a somewhat different form of phase equilibria from [10] is presented in the region of Ag– Ag_2Se – Ag_8SnSe_6 – SnSe –Sn compositions. According to the analysis of [13] and [15], in the state diagram constructed in [10] 5 monovariant phase equilibria converge at two nonvariant points, which contradicts the phase rule, and there is a field on the liquidus surface projection that cannot be attributed to the primary crystallization phase system.

The crystallographic data of the ternary compounds Ag_8SnSe_6 and AgSnSe_2 are presented in [1, 14–17]. The high-temperature modification of Ag_8SnSe_6 crystallizes in a cubic lattice (space group $F-43m$) with a period $a = 1.112$ nm [14], and low-temperature in an orthorhombic (space group $Pmn2_1$) with parameters $a = 0.79168$ (6), $b = 0.78219$ (6), $c = 1.10453$ (8) nm [16]. The phase of variable composition based on AgSnSe_2 has a cubic structure of the NaCl type, the lattice period for the stoichiometric composition is $a = 0.5627$ nm [17].

Due to the inconsistency of literature data on phase equilibria in the Ag–Sn–Se system, the phase diagram was thoroughly studied in [15]. In this work, based on the study of the phase diagrams quasibinary sections Ag_2Se – SnSe_2 , Ag_2Se – SnSe , Ag_8SnSe_6 – SnSe ,

Ag_8SnSe_6 – Se and polytermic incisions AgSe – SnSe , Ag_2Se – 3Sn Ag– SnSe , AgSn – Se received new refined phase diagram system

Ag–Sn–Se (Figure 1, 2), somewhat different from those previously given in the literature. It was shown that two ternary compounds Ag_8SnSe_6 and AgSnSe_2 are formed in the system, melting congruently at 1015 K and incongruently at 860 K, respectively. Earlier in the above literature ternary compound Ag_2SnSe_3 not confirmed. Based on the phase diagrams of the boundary binary systems using a limited number of DTA data, 3D modeling and visualization of the liquidus surfaces and immiscibility in the Ag–Sn–Se ternary system was carried out. For the calculation and 3D modeling, the analytical method proposed and tested in [18–20] was used.

Fig. 1. Isothermal section of the Ag–Sn–Se system at 300 K [15]: greek letters denote solid solutions based on Ag (α), high-temperature modification Ag_2Se (α') and AgSnSe_2 (γ) and also intermediate phases in the Ag–Sn system (ξ , ϵ). Indexes I and II refer to low-temperature and high-temperature modifications of the compound, respectively.

Fig. 2. Projection of the liquidus surface and immiscibility in the Ag–Sn–Se system [15]. Primary crystallization fields: 1 – solid solutions based on Ag; 2,3–intermediate phases in the Ag–Sn system; 4 – high temperature modification of Ag_2Se ; 5– SnSe (I, II); 6 – SnSe_2 ; 7 – Ag_8SnSe_6 (II); 8 – AgSnSe_2 ; 9 – Sn; 10 – Se. Indexes I and II refer to low-temperature and high-temperature modifications of the compound, respectively.

Fig. 3. The orthorhombic structure of $\beta\text{-Ag}_8\text{SnSe}_6$ with the space group $Pmn2_1$ (a). The cubic structure of $\gamma\text{-Ag}_8\text{SnSe}_6$ with the space group $F\bar{4}3m$. (b). The cubic structure can be considered as Se^{2-} anions forming a cubic frame with four Se^{2-} and four tetrahedral $[\text{SnSe}_4]^{4+}$ units inside the tetrahedral voids (c). Ag^+ ions are delocalized over the entire cubic structure. Green spheres indicate selenium, medium violet indicates tin, and fully filled and partially filled red spheres indicate Ag^+ (d).

In [1], using the sintering technology in a hot press, a γ -Ag₈SnSe₆-*n*-type superionic semiconductor compound was synthesized, which is a promising thermoelectric material up to 550°C. It was revealed that β -Ag₈SnSe₆ has an orthorhombic structure with the space group $Pmn2_1$ and is not a superionic conductor (Figure 3a). At the same time, the γ -phase with superionic conductivity has a face-centered cubic structure with a space group of $F\bar{4}3m$ (Figure 3b).

It was also found in [1] that the $\beta \leftrightarrow \gamma$ structural transition occurs between 80°C and 90°C (Figure 4).

Fig. 4. TG–DSC curves showing the $\beta \leftrightarrow \gamma$ phase transition at 83°C and melting/decomposition at 700°C [1].

Thermodynamics

In [1] it was revealed that the thermal conductivity of the γ -phase Ag₈SnSe₆ at temperatures above is below the glass limit, for the

reason that the heat capacity C_V and C_p is less than $3Nk_B$ (N is Avogadro number and k_B is Boltzmann constant) and this phase has ultra-low thermal diffusion coefficient (Figure 5).

From Figure 5b it follows that $C_p = C_V$. At analyzing the data in Figure 5b, the question arose about the dimension C_p (C_V) on the ordinate. According to the Dyulong-Petit formula for one mol-atom of the compound $C_p = 3N_A k_B = 24.96 \text{ J/(mol-atom K)}^{-1}$. This indicates that the values of heat capacity on the ordinate of Figure 5b refer to one mole-atom of the Ag₈SnSe₆ compound and are presented in $C_p \cdot 10^{-2}$. Then from the graph in Figure 5b for $T = 298 \text{ K}$ we can write $C_{p,298}(\text{Ag}_8\text{SnSe}_6) = 0.26 \cdot 100 \cdot 15 = 390 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$. Here 15 is the number of atoms in the Ag₈SnSe₆ molecule. According to the Dyulong-Petit $C_{p,298}(\text{Ag}_8\text{SnSe}_6) = 374 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$. The molar heat capacity of Ag₈SnSe₆ was also calculated using the methods of Kubashevsky and Ivanova, previously successfully tested in [21–25]. When applied to the Ag₈SnSe₆ compound, the Ivanova equation [23] has the form:

$$C_{p,298}(\text{Ag}_8\text{SnSe}_6) = m(22.14 + 2480/T_m) \quad (1)$$

$m = 15$, $T_m(\text{Ag}_8\text{SnSe}_6) = 1015 \text{ K}$ [5]. Then from (1) it follows that $C_{p,298}(\text{Ag}_8\text{SnSe}_6) = 368.7$.

Fig. 5. Data for γ -Ag₈SnSe₆ [1]: (a) $C_p(T)$ and $C_V(T)$ dependences. Data for high T , for clarity, is given in (b). The dashed dark yellow line and the dashed green line indicate the Dulong-Petit limit for C_p and the lowest theoretical C_p value, respectively. In (c), the diffusion coefficient D is shown as a function of temperature, and the total thermal conductivity (k_{tot}) and the maximum thermal conductivity of the crystal lattice (k_{min}) are presented in the graph (d).

It follows from the calculations that, on the one hand, the dimension of the heat capacity on the ordinate in Figure 5b is indicated incorrectly; on the other hand, the experimental values of the heat capacity of Ag_8SnSe_6 obtained in [1] are reliable. The thermodynamic data of silver, tin, and ternary selenides are systematized in Table 1.

In binary side systems Ag–Se and Sn–Se of the ternary system Ag–Sn–Se, there are wide areas of homogeneity that propagate inside the concentration (Figure 2) triangle. For the calculation and approximation of the free energy of mixing liquid solutions, an asymmetric version of the model of regular solutions, successfully tested in [35–38], was used:

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

where ΔG_T^0 – free energy of mixing of liquid solutions, the first term – entropy of mixing liquid solutions, the second term – entropy of mixing, $R = 8.314 \text{ J mol}^{-1} \cdot \text{K}^{-1}$).

Equation (1) is solved on the basis of the Baevsky Bayesian approximation [39]. To deter-

mine the immiscibility boundary, the thermodynamic condition of internal stability is used:

$$(\partial^2 \Delta G^0 / \partial x^2)_{P,T} > 0 \quad [40].$$

The second derivative of the Gibbs free energy (2) is defined as follows.

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

The second derivative is determined using the online program [46]. The dependences of the function (3) for temperatures of 900, 950, 1000, 1050, and 1080 K are shown in Figure 6.

As a result of thermodynamic calculations, it was revealed that the critical solubility temperature in the Ag–Se system is equal to $T = 1080 \text{ K}$. In this temperature in the concentration range $X_{\text{Se}} = 0.45 \div 0.95$, the function of internal stability is greater than zero $(\partial^2 \Delta G^0 / \partial x^2)_{P,T} > 0$. The dependence of the temperature for the separation boundary on the composition is approximated by the equation

$$T, \text{ K} = -6887.39418 + 42972.06249x - 87204.80219x^2 + 79466.09268x^3 - 27593.75741x^4$$

Standard thermodynamic functions of silver, tin and ternary selenides

Phase	$-\Delta G_f^0, 298$ kJ/mol	$-\Delta H_f^0, 298$ kJ/mol	$\Delta S_f^0, 298$ J/(mol.K)	$C_p^0, 298$ J/(mol.K)	Source
$\gamma\text{-Ag}_8\text{SnSe}_6, *$	352.5 ± 1.9	323.1 ± 1.6	98.6 ± 3.1	378.5 ± 3.5	[25, 26] [1]
AgSnSe_2	133.9 ± 1.6	124.9 ± 1.3	30.1 ± 2.5		[25, 26]
$\beta\text{-Ag}_2\text{Se}$	59.3 ± 0.6	51.9 ± 0.5	25.1 ± 0.9	81.75 ± 0.42	[25, 26] [27, 28]
SnSe	90.3 ± 1.9	77.8 ± 1.7	42.3 ± 3.2	49.06 ± 0.5	[25] [29]
SnSe	96.3 ± 0.4	94.6 ± 2.1	5.0 ± 1.6		[24]
SnSe_2	77.3 ± 2.5	82.4 ± 4.5	-17.2 ± 2.5	76.7 ± 5 73.39 ± 0.8	[24] [29]
AgSnSe_2	146.4 ± 0.5	148 ± 3	-5.37 ± 1.5		[30, 31]
$\gamma\text{-Ag}_8\text{SnSe}_6$	350.3 ± 1.8	320.4 ± 8.1	100.35 ± 8.5		[30, 31]
$\beta\text{-Ag}_2\text{Se}$	47.6 ± 1.5	35.0 ± 2.5	42.21 ± 0.5		[32]
$\beta\text{-Ag}_2\text{Se}$	47.6 ± 0.1	35.1 ± 0.1	42.18 ± 0.2		408–500 K [33]

$\gamma\text{-Ag}_8\text{SnSe}_6, *$ – thermodynamic functions of this phase are determined by extrapolation of the EMF data measured in the interval 480–560 K.

Fig. 6. The dependence of the internal stability function of Gibbs on the mole fraction of selenium for liquid alloys of the Ag–Sn–Se system in the composition range $x_{\text{Se}} = 0.45 \div 0.95$. (All functions are presented in the version for computer programs):

$$\begin{aligned}
 & -2 \cdot (16000 - 10000 \cdot x^2 - 2 \cdot 10000 \cdot x \cdot (x-1) - 10000 \cdot x \cdot (3 \cdot x-1)) + 8.31 \cdot 1080 / (1-x) + 8.31 \cdot 1080 / x \\
 & -2 \cdot (25000 - 10000 \cdot x^2 - 2 \cdot 10000 \cdot x \cdot (x-1) - 10000 \cdot x \cdot (3 \cdot x-1)) + 8.31 \cdot 1050 / (1-x) + 8.31 \cdot 1050 / x \\
 & -2 \cdot (40000 - 12000 \cdot x^2 - 2 \cdot 12000 \cdot x \cdot (x-1) - 12000 \cdot x \cdot (3 \cdot x-1)) + 8.31 \cdot 1000 / (1-x) + 8.31 \cdot 1000 / x \\
 & -2 \cdot (50000 - 12000 \cdot x^2 - 2 \cdot 12000 \cdot x \cdot (x-1) - 12000 \cdot x \cdot (3 \cdot x-1)) + 8.31 \cdot 950 / (1-x) + 8.31 \cdot 950 / x \\
 & -2 \cdot (70000 - 10000 \cdot x^2 - 2 \cdot 10000 \cdot x \cdot (x-1) - 10000 \cdot x \cdot (3 \cdot x-1)) + 8.31 \cdot 900 / (1-x) + 8.31 \cdot 900 / x
 \end{aligned}$$

Similar equations were obtained for other phase regions and used for analytical 3D modeling of the crystallization surface and separation of liquid solutions of the Ag–Sn–Se system (Figure 7).

Modeling

The use of a genetic algorithm with Bayesian statistics makes it possible to efficiently and meaningfully combine uncertain data sets, both large and small [39]. This process then leads to the optimization of the parameters of the proposed models and the assessment of the overall forecast confidence in these models. In particular, this work determines the degree of uncertainty at the interphase boundaries of the crystallization surface of SnSe, SnSe₂, Ag₂Se, Ag₈SnSe₆ compounds in the Ag–Sn–Se ternary system, taking into account the available data on boundary phases, accepted models of interphase boundaries and thermodynamic data used in these models. The end result was a general reduction in the uncertainty of the thermodynamic data values, as well as the position of the phase boundary. The use of modern heuristic optimizers, such as ge-

netic algorithms, is crucial for this work, as they are both reliable and do not require any assumptions about the forms of distribution of uncertainty. Based on the phase diagrams of boundary binary systems and a limited number of DTA data from samples of the ternary system using the OriginLab program using the Bayesian statistics method [39], equations describing the surfaces of the primary crystallization of Ag₂Se, SnSe₂, SnSe, Ag₈SnSe₆ and delamination in the Ag–Sn–Se system were obtained. Using these equations, 3D visualization of these surfaces is carried out.

For 3D modeling of the surfaces of monovariant equilibria in the 1–2–3 ternary system, the temperature dependences of the composition are determined as an explicit function $T = f(x, y)$, where the x – atomic fraction of the basis component, say component 1. Let us assume that $x = X_1$, then $y = Y = Y = X_2 / (X_2 + X_3)$. This method of analytical 3D modeling of the surfaces of monovariant equilibria of ternary systems was successfully tested on specific systems and described in detail in [41–43]. In this paper, the belowfollowing analytical expressions were obtained for the Ag₂Se, SnSe₂, SnSe, Ag₈SnSe₆

crystallization surfaces and delamination surfaces in the Ag–Sn–Se system.

For the surface of crystallization of Ag_2Se , in the concentration range $X=0.31\div0.42$, $Y=0\div0.16$:

$$T, K = [107558 - 531117(1-X) + 875875(1-X)^2 - 477852(1-X)^3](1-Y)^{1.06}. \quad (4)$$

For the surface of crystallization of SnSe , in the concentration range $X=0.5\div0.61$, $Y=0.36\div1$.

$$T, K = (349 + 4829X - 6436X^2)Y^{0.28}. \quad (5)$$

For the surface of crystallization of SnSe_2 , in the concentration range $X=0.61\div0.95$, $Y=0.52\div1$.

$$T, K = (-979787.7 + 7.75995 \cdot 10^6 X - 2.55035 \cdot 10^7 X^2 + 4.45533 \cdot 10^7 X^3 - 4.36243 \cdot 10^7 X^4 + 2.26954 \cdot 10^7 X^5 - 4.90063 \cdot 10^6 X^6)Y^{0.35}. \quad (6)$$

For the surface of crystallization of Ag_8SnSe_6 , in the concentration range $X=0.35\div0.55$, $Y=0.135\div0.62$.

$$T, K = 802 + 2044Y - 6091Y^2 + 4237Y^3 - 4049 + 26685X - 57428X^2 + 40000X^3. \quad (7)$$

For surface immiscibility from Sn–Se ($X=0.16\div0.49$; $Y=0.33\div1$).

$$T, K = (-1729 + 37308X - 173477X^2 + 357612X^3 - 275627X^4)Y^{0.38}. \quad (8)$$

For surface immiscibility from Ag–Se ($X=0.12\div0.31$, $Y=0\div0.33$).

$$T, K = (-4057 + 104175X - 753245X^2 + 2.40816 \cdot 10^6 X^3 - 2.87183 \cdot 10^6 X^4)(1-Y) \quad (9)$$

For surface immiscibility from Ag–Se ($X=0.44\div0.98$, $Y=0\div0.53$).

$$T, K = (-9582 + 60199X - 127181X^2 + 119250X^3 - 41950X^4)(1-Y)^{0.4}. \quad (10)$$

In the equations (4–10): $X=X_{\text{Se}}$, $Y=X_{\text{Sn}}/(X_{\text{Sn}}+X_{\text{Ag}})$, X_{Ag} , X_{Sn} , X_{Se} – atomic fractions of components in liquid alloys of the Ag–Sn–Se system; the $f(X)$ polynomials are determined on the basis of the liquidus curves of the compounds and the separation curves of double Ag–Se and Sn–Se boundary systems; The parameters associated with the change in Y are determined on the basis of a limited number of DTA data from samples of the ternary system and the Ag_2Se – SnSe and Ag_2Se – SnSe_2 quasi-binary sections.

Fig. 7. Multi 3D model of Ag_2Se , SnSe_2 , SnSe , Ag_8SnSe_6 crystallization surfaces and immiscibility surfaces in the Ag–Sn–Se system.

These analytical expressions with sufficient accuracy explicitly link the liquidus temperatures and the compositions of the components of the ternary system and allowed the task of 3D visualization of the surfaces of crystallization of compounds and delamination in the system of the Ag–Sn–Se system (Figure 7).

Conclusion

As a result of the analysis and systematization of literature information, it was revealed that there are reliable data for the phase diagram, the thermodynamic functions of formation and the structure of ternary compounds in the Ag–Sn–Se system, which are used to determine the conditions for the materials synthesis of having mixed ion-electron conductivity in combination with high thermoelectric and optical properties, superconductivity. Modern computer programs are used for the thermodynamic calculation and simulate phase equilibria in the Ag–Sn–Se system. Based on the phase diagrams of the boundary binary systems using a limited number of DTA data, using the computer program OriginLab, analytical expressions were obtained with sufficient accuracy in the explicit form of connecting the liquidus temperatures and the compositions of the components of the ternary system. The 3D visualization problem for Ag_2Se , SnSe_2 , SnSe , Ag_8SnSe_6 crystallization surfaces and delamination surfaces in the Ag–Sn–Se system was solved on the same graph.

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СИСТЕМА Ag–Sn–Se: ФАЗОВАЯ ДИАГРАММА, ТЕРМОДИНАМИКА И МОДЕЛИРОВАНИЕ

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Проведен сравнительный анализ работ по исследованию фазовых равновесий, структур и термодинамических свойств промежуточных фаз тройной системы Ag–Sn–Se. Показано, что в системе образуется два тройных соединения – Ag_8SnSe_6 и AgSnSe_2 , плавящиеся конгруэнтно при 1015 К и инконгруэнтно при 860 К, соответственно. Рекомендованы наиболее достоверные данные для энтальпии, энтропии, свободной энергии образования и теплоемкостей AgSnSe_2 и аргиродитной фазы Ag_8SnSe_6 . Термодинамические функции смешения жидких растворов аппроксимированы в рамках асимметрического варианта модели регулярных растворов. Для определения границ расслоения жидких сплавов использована функция внутренней термодинамической стабильности гомогенной фазы. С помощью программы OriginLab2018 проведена мульти 3D визуализация поверхностей кристаллизации Ag_2Se , SnSe_2 , SnSe , Ag_8SnSe_6 и поверхностей расслаивания в системе Ag–Sn–Se.

Ключевые слова: система медь–свинец–теллур, фазовая диаграмма, поверхность ликвидуса, 3D моделирование.

Ag–Sn–Se SİSTEMİ: FAZA DİAQRAMI, TERMODİNAMİKA VƏ MODELƏŞMƏ

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Ag–Sn–Se üçlü sisteminin faza diaqramının, aralıq fazalarının strukturlarının və termodinamik xassələrinin öyrənilməsi üzrə işlərin müqayisəli təhlili aparılmışdır. Sistemdə Ag_8SnSe_6 və AgSnSe_2 üçlü birləşməsinin əmələ gəlməsi, onların müvafiq olaraq 1015 K-də parçalanmadan əriməsi və 860 K-də parçalanaraq əriməsi müəyyən edilmişdir. AgSnSe_2 və argirodit Ag_8SnSe_6 birləşmələrinin əmələgəlmə enthalpiya, entropiya, sərbəst enerjiləri və istilik tutumları üçün ən etibarlı məlumatlar təklif olunur. Maye ərintilərin qarışma termodinamik funksiyaları müntəzəm məhlullar modelinin asimmetrik versiyası əsasında ifadə edilir. Maye ərintilərin təbəqələşmə sərhədlərini müəyyən etmək üçün homogen fazanın daxili termodinamik sabitlik funksiyasından istifadə edilmişdir. OriginLab proqramın köməyi ilə Ag–Sn–Se sistemindəki Ag_2Se , SnSe_2 , SnSe , Ag_8SnSe_6 birləşmələrinin kristallaşma səthləri və maye ərintilərinin təbəqələşmə səthlərinin çoxsəhəli 3D görüntüsü verilmişdir.

Açar sözlər: mis–qurğuşun–tellur sistemi, faza diaqramı, lividus səthi, 3D modelləşdirilmə.