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3D ANALYTICAL MODELING OF CRYSTALLIZATION SURFACES OF THE MnTe–SnTe–Sb₂Te₃ SYSTEM

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An analytical method was used for 3D modeling of crystallization surfaces of the MnTe–SnTe–Sb₂Te₃ system based on the existing data of boundary systems and a small number of experimental DTA-measurements. All analytical dependencies temperatures on composition for liquidus of the binary and three-system were obtained using the 2D and 3D options of the OriginLab software. The obtained results allowed us to visualize the crystallization surfaces of the phases based on initial components of the MnTe–SnTe–Sb₂Te₃ system as a separate form and in one graph.

Keywords: 3D analytical modeling, liquidus surfaces, MnTe–SnTe–Sb₂Te₃ system, topological insulators.

doi

Introduction

Tetradymite-type layered ternary phases of the quasi-binary A^{IV} (A^{VII}) Te–B₂^V Te₃ (A^{IV} = Ge, Sn, Pb; A^{VII} = Mn; B₂^V = Sb, Bi) systems have been intensively studied as three-dimensional topological insulating materials [1–5]. Among them manganese contained layered phases have especially gained substantial attention since MnBi₂Te₄ and other ternary manganese-bismuth tellurides possess both topological insulating (TI) and magnetic properties at the same time [6–14]. The relationship between magnetism and TI behavior has dramatically inspired great attention in recent years due to their potential prospects to realize many interest topological phenomena, including quantum anomalous Hall Effect, topological axion insulators, etc. More recent investigations indicated to the existence of layered chalcogenide MnSb₂Te₄ which is a structural analog of the well-known MnBi₂Te₄, is an antiferromagnetic semiconductor with a trivial energy gap [15–17]. In this connection, layered manganese antimony (or bismuth) tellurides and phases based on them with partial substitution of manganese with other elements can be a platform for experimental visualization of many annown yet topological quantum effects.

The phase relationship in the MnTe–SnTe–Sb₂Te₃ system was studied by us using powder XRD, DTA, and SEM results of the equilibrated alloys. In this work, an analytical method was used for 3D modeling of crystallization surfaces of the MnTe–SnTe–Sb₂Te₃ system based on the data of boundary systems and a small number of experimental DTA measurements. All analytical dependencies were obtained using the "analysis" option of the OriginLab software.

Modeling technique

An analytical method was used for the 3D modeling of crystallization surfaces of the MnTe–SnTe–Sb₂Te₃ system. The method was successfully tested in several works up to now [18–23]. The temperature dependences of the crystallization surface were determined as a form of function (1) for the three-component MnTe–SnTe–Sb₂Te₃ system:

$$T=f(x, y). \quad (1)$$

Here x – is the mole fraction of MnTe: $y=x(\text{Sb}_2\text{Te}_3/[x(\text{Sb}_2\text{Te}_3)+x(\text{SnTe})]$ and y – is relative mole fraction of Sb₂Te₃ in MnTe–SnTe–Sb₂Te₃ system.

The obtained analytical expressions for ternary MnTe–SnTe–Sb₂Te₃ and its boundary systems are listed in Tables 1 and 2. All analyt-

ical dependences were presented in the form used by the OriginLab software.

The modeling process was carried out in the following order. Firstly, the temperature dependences of the compositions were determined as $T = f(x)$ and $T = f(y)$ for the liquidus of each boundary system. Next, $T = f(x, y)$ function was defined based on experimental results of the MnTe–SnTe–Sb₂Te₃ system.

Results and discussion

Binary boundary systems. The boundary systems of the investigated system have been carefully studied. The phase equilibria of the MnTe–Sb₂Te₃ system was investigated using powder X-ray diffraction and Differential Thermal Analysis methods in [24]. The system is featured with the formations of 2 intermediate compounds, MnSb₂Te₄ and MnSb₄Te₇, which melts peritectically at 920 and 901 K respectively. There are significant solid-solubility fields based on both ternary compounds and starting Sb₂Te₃. Similarly, the SnTe–Sb₂Te₃ system is also featured by the formation of the two ternary SnSb₂Te₄ and SnSb₄Te₇ compounds that melt peritectically at 868 and 866 K respectively. Besides, the system has homogeneity areas

based on both starting and intermediate compounds. However, the SnTe–MnTe system is characterized by a wide range of solid solutions based on SnTe and MnTe [25].

The phase diagrams of the boundary SnTe–MnTe, MnTe–Sb₂Te₃ and SnTe–Sb₂Te₃ systems and their analytical dependences for liquidus curves are shown in Table 1 (eq.1–10). Analytical dependencies were determined using the "analysis" option of the OriginLab software. As can be seen in Figure 1, obtained analytical dependence approximates the liquidus curve of the compound of the MnTe–Sb₂Te₃ system with sufficient accuracy.

MnTe–SnTe–Sb₂Te₃ system. The analytical dependences for 3D modeling of the liquidus surfaces of the MnTe, SnTe, and Sb₂Te₃ phases are given in Table 2 (equations 11–14). These equations allowing us to visualize the crystallization surfaces separately (Figure 5) and on one graph of all phases (Figure 6).

The crystallization surfaces of phases based on initial components of the MnTe–SnTe–Sb₂Te₃ system are visualized in Figure 6, where the 3D phase diagram of the system is viewed from the side of the MnTe–Sb₂Te₃ system, from top to bottom.

Fig. 1. Dependence of the liquidus temperatures of the MnTe compound on the composition in the MnTe–Sb₂Te₃ system: curve – polynomial, symbols – experimental results taken from [24].

Table 1. Phase diagrams and analytical dependencies of their liquidus curves of the SnTe–MnTe, MnTe–Sb₂Te₃, and SnTe–Sb₂Te₃ systems (equations are presented in computer variation)

Phase diagram	Region	Equations: T,K=f(x)	Eq.N.
<p>Fig. 2. Phase diagram of the MnTe-Sb₂Te₃ system [24].</p>	liquidus (Mn ht), $x=x(\text{MnTe})=0.93\div 1$	$1250+186*x$	1
	liquidus (MnTe ht,it ₁ , it ₂ , rt), $x=x(\text{MnTe})=0.255\div 0.93$	$-190+6990*x-12819*x^2+10983*x^3-3521*x^4$	2
	curve p ₁ p ₂ $x=x(\text{MnTe})=0.2\div 0.255$	$652,64+1944,85*x-3515,15*x^2$	3
	curve p ₂ e $x=x(\text{MnTe})=0.154\div 0.25$	$746,13+1384,7*x-3051,84*x^2$	4
	liquidus (β-Sb ₂ Te ₃) $x=x(\text{MnTe})=0\div 0.154$	$893-9,907*x-188,66*x^2$	5
<p>Fig. 3. Phase diagram of the SnTe-Sb₂Te₃ system.</p>	Liquidus (α-SnTe), $x=x(\text{Sb}_2\text{Te}_3)=0\div 0.55$	$1080,6-614,3*x+190,9*x^2+409,2*x^3$	6
	Liquidus (β-Sb ₂ Te ₃ , $x=x(\text{Sb}_2\text{Te}_3)=0.61\div 1$	$729,92+316,92*x-153,85*x^2$	7
<p>Fig. 4. Phase diagram of the SnTe-MnTe system [25].</p>	Liquidus (Mn ht),, $x=x(\text{MnTe})=0.91\div 1$	$928+544*x$	8
	Liquidus (MnTe), $x=x(\text{MnTe})=0.25\div 0.91$	$1272-2444*x+10388*x^2-14994*x^3+7390*x^4$	9
	Liquidus (α-SnTe), $x=x(\text{MnTe})=0\div 0.25$	$1070+237*x-390*x^2$	10

Table 2. Analytical dependencies for crystallization surfaces of phases based on initial components of the MnTe–SnTe–Sb₂Te₃ system

Liquidus surface, region	$T, K = f(x, y);$ $x = x(\text{MnTe}); y = x(\text{Sb}_2\text{Te}_3) / [x(\text{Sb}_2\text{Te}_3) + x(\text{SnTe})];$ $x_i = \text{mole fractions MnTe, SnTe, Sb}_2\text{Te}_3$	Eq. N
(Mn ht), $x = x(\text{MnTe}) = 0.91 \div 1;$ $0.93 \div 1; y = 0 \div 1$	$(1250 + 186 * x) * y + (928 + 544 * x) * (1 - y)$	11
liquidus (MnTe ht, it ₁ , it ₂ , rt), $x = x(\text{MnTe}) = 0.245 \div 0.91;$ $y = 0 \div 1$	$(-190 + 6990 * x - 12819 * x^2 + 10983 * x^3 - 3521 * x^4) * y + (1272 - 2444 * x + 10388 * x^2 - 14994 * x^3 + 7390 * x^4) * (1 - y)$	12
liquidus (α -SnTe), $x = x(\text{MnTe}) = 0 \div 0.29;$ $y = 0 \div 0.56$	$(1080.6 - 614.3 * y + 190.9 * y^2 + 409.2 * y^3) * (1 - x)^{-0.112}$	13
liquidus (β -Sb ₂ Te ₃), $x = x(\text{MnTe}) = 0 \div 0.295;$ $y = 0.33 \div 1$	$(729.92 + 316.92 * y - 153.85 * y^2) * (1 - x)^{0.04}$	14

Fig. 5. 3D model of crystallization surface of phase based on MnTe, visualized by the equation (12) Table 2.

Fig. 6. Multi-3D model of crystallization surfaces of phases based on (Mn ht), (MnTe ht, it₁, it₂, rt), α -SnTe and β -Sb₂Te₃ in the MnTe–SnTe–Sb₂Te₃ system, visualized by equations 11–14 in Table 2.

Conclusion

An analytical method was used for 3D modeling of crystallization surfaces of the MnTe–SnTe–Sb₂Te₃ system based on the data of boundary systems and a small number of experimental DTA-measurements. The obtained analytical dependences of the liquidus temperatures on the composition allowed us to visualize the crystallization surfaces of phases based on initial components of the MnTe–SnTe–Sb₂Te₃ system as a separate form and in one graph. All analytical dependences were obtained using the 2D and 3D analytical options of the OriginLab software. Matrices in the form of $100 \times 100 = 10.000$ and $50 \times 50 = 2500$ tabular data can be used for choosing the optimal values of the composition and temperature for the synthesis of binary alloys, as well as alloys of the MnTe–SnTe–Sb₂Te₃ system.

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MnTe–SnTe–Sb₂Te₃ SİSTEMİNDƏ KRİSTALLAŞMA SƏTHLƏRİNİN 3D ANALİTİK MODELƏŞDİRİLMƏSİ

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MnTe–SnTe–Sb₂Te₃ sisteminin kənar ikili sistemlərinin faza diaqramları və seçilmiş bir neçə tərkibin DTA nəticələrinə əsasən üçlü sistemin kristallaşma səthlərinin 3D modelləşdirilməsi üçün analitik asılılıqlar müəyyənləşdirilmişdir. Asılılıqların təyini üçün OriginLab proqramının 2D və 3D modelləşdirmə funksiyalarından istifadə olunmuşdur. Təyin edilmiş temperatur-tərkib analitik asılılıqları vasitəsi ilə MnTe–SnTe–Sb₂Te₃ sisteminin fazalarının kristallaşma səthlərinin 3D görüntüsünü alınmışdır

Açar sözlər: 3D analitik modelləşdirmə, kristallaşdırma səthləri, MnTe–SnTe–Sb₂Te₃ sistemi, topoloji izolyatorlar.

3D АНАЛИТИЧЕСКОЕ МОДЕЛИРОВАНИЕ КРИСТАЛЛИЗАЦИОННЫХ ПОВЕРХНОСТЕЙ СИСТЕМЫ MnTe–SnTe–Sb₂Te₃

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Для трехмерного моделирования поверхностей кристаллизации системы MnTe–SnTe–Sb₂Te₃ использовался аналитический метод на основе имеющихся данных граничных систем и небольшого количества экспериментальных ДТА-измерений. Аналитические зависимости температур от составов для ликвидусов исследуемой тройной системы и граничных бинарных систем получены с использованием 2D и 3D функции программы OriginLab. Полученные результаты позволили визуализировать поверхности кристаллизации фаз системы MnTe–SnTe–Sb₂Te₃.

Ключевые слова: трехмерное аналитическое моделирование, поверхности ликвидуса, система MnTe–SnTe–Sb₂Te₃, топологические изоляторы.