THE EQUATION FOR LIQUIDUS LINE OF THE In_2Te_3-Co_3Te_4 SYSTEM PHASE DIAGRAM

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The equation for a calculation of the liquidus line of the In_2Te_3-Co_3Te_4 system state diagram was derived. With this purpose, the liquidus line, consisting of two branches, was accepted to be similar to branches of two parabolas, that is why the parabola equation was used for the derivation of the mathematical expression. Using the suggested equation, content values and fusion temperatures of interacting components may be calculated with high accuracy, in the broad concentration interval.

The phase state diagram of the system In_2Te_3-Co_3Te_4 was earlier constructed on the base of the experimental data of the complex of physico-chemical analysis methods [1] and it was revealed, that on curves of the alloy thermogram heating, concentrated by In_2Te_3, the effects, connected with the polymorphic transformation of the ordered modification α-In_2Te_3 into the unordered β-In_2Te_3, are clearly manifested. It was also established, that the temperature of the phase transition α- In_2Te_3 into β- In_2Te_3 increases from 890 K up to 960 K under the influence of Co_3Te_4 and the dependence of the phase transition temperature on the concentration occurs here. Therefore, the confirmation of figure points coordinates of the state diagram of this system by theoretical calculations is an actual one.

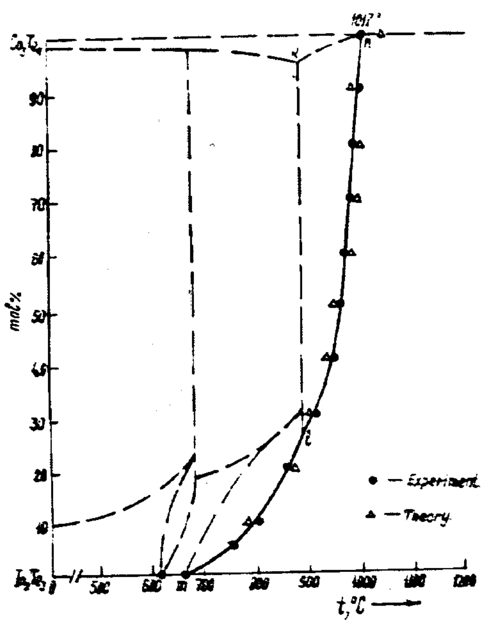

Fig.1. The part of the state diagram of the system In_2Te_3-Co_3Te_4 in the high temperature region.

There are a number of works, devoted to thermodynamic calculations of liquidus line of binary and more complicated systems. However, there is no information about mathematical calculations. The authors of [2] made an attempt to receive the restriction equation for the calculation of binodile stratification curves in systems Hg-Tl_2X (where X=S, Se, Te). The results of the derivation of the equation for the liquidus curve plotting and boundaries determination of the phase formation reaction in the system In_2Te_3-Co_3Te_4 are given in the present report. Main lines fragments of the phase interface of the system In_2Te_3-Co_3Te_4 are presented on fig.1. For clarity the scheme was constructed in the form of the dependence x-$f(t)$, where x is the crystal content, t is the temperature (the content is meant through U in the derived equations). The liquidus lines on the state diagram may be observed as branches of two parabolas. One branch (***nl*** line) is the part of the large parabola, the other (***ml*** line) is the half of the smaller parabola. Therefore, analytical expressions of ordinary parabolas served the base for worked out equations of liquidus lines. The analysis of the results of the undertaken research showed, that the change of the substance transformation rate versus the temperature may be described by the following linear differential equation [3].

$$\frac{dU(t)}{dt} = (a+bt)U(t), \tag{1}$$

where $U(t)$ describes the substance state versus the temperature, a and b are parameters, characterizing the influence of the temperature change on the substance state. It is necessary to note, that the equation (1) is observed with the initial condition:

$$U(t_0) = U_0 \tag{2}$$

It is necessary to solve (1) with the initial condition (2) for determination of the change degree of the substance state. Let us rewrite (1) as

$$\frac{dU(t)}{U(t)} = (a+bt)dt \tag{3}$$

and suggest, that $t_0=0$. The solution of the equation (3) with the initial condition $U(0)=U_0$ looks as:

$$bt^2 + 2at - 2\ln\left[\frac{U(t)}{U_0}\right] = 0 \tag{4}$$

Calculating the quadratic equation (4), we obtain t as the function of U

$$t(U) = \frac{-a \pm \sqrt{a^2 + 2b\ln\left[\frac{U(t)}{U_0}\right]}}{b} \tag{5}$$

Now if:

1. $a^2 + 2b\ln\left[\frac{U(t)}{U_0}\right] = 0$, then it follows from (5), that

$t(U) = -\frac{a}{b}$ $(a>0, b<0)$, i.e. in this case $t(U) = -\frac{a}{b} = const > 0$.

2. $a^2 + 2b\ln\left[\frac{U(t)}{U_0}\right] > 0$, i.e. $a^2 > -2b\ln\left[\frac{U(t)}{U_0}\right]$, or $|a| > \sqrt{-2b\ln\left[\frac{U(t)}{U_0}\right]}$, where $b<0$. In this case the function $t(U)$ has two representations, namely:

$$t_1(U) = \frac{-a + \sqrt{a^2 + 2b\ln\left[\frac{U(t)}{U_0}\right]}}{b}$$
$$t_2(U) = \frac{-a - \sqrt{a^2 + 2b\ln\left[\frac{U(t)}{U_0}\right]}}{b} \qquad (6)$$

At all parameters values $a>0$, $b<0$ or $a<0$, $b>0$ the function (9) is positive. It is possible to apply the simple polynomial equation for determination of concrete values of "a" and "b". The most suitable method of these parameters determination is the method of the least squares. However, it is possible to use more simple method for our case, for example: the method of means. Guided by this method and having divided the liquidus line into 2 temperature intervals (the first interval spreads to ml line, the second to nl), we determined the "a" and "b" parameters values . In fact, on the experimentally constructed diagram of the liquidus line there is a break at the beginning of the peritectoid transformation (lk line). For the interval 667<t<917°C it has been found from the calculation of means, that $a=-3\cdot10^{-3}$ (degree^{-1}), $b=9.7\cdot10^{-6}$ (degree^{-2}). In this case, the equation (4) will take a form

$$LnU - lnU_0 = b/2t^2 + at$$

or

$$U = U_0 exp(at + b/2t^2)$$
$$U = exp(-3\cdot10^{-3}t + 4.87t^2)$$

The equation was observed with the initial conditions $U_0=U(667)=1$.(The unit reflects the initial components content, i.e In_2Te_3 without Co_3Te_4 admixture).

It was found for the temperature interva l917<t<1017°C, that $a=-2.7\cdot10^{-2}$ (degree^{-1}), $b=4.2\cdot10^{-5}$ (degree^{-2}). Consequently, $lnU=ln\ 100-2.7\cdot10^{-2}\ t+2.1\cdot10^{-5}t^2$, with the regard of the initial condition $U(t_0) = U(1017)=100$, i.e. the approach start was taken from the Co_3Te_4 side).

The experimental and calculated values of fusing temperature and content of system alloys In_2Te_3-Co_3Te_4.

Table 1

Experiment		Calculation	
Content mole %	Temperature °C	Content mole %	Temperature °C
10	792	10.2	788
20	877	19.7	878
30	927	29.9	926
40	972	39.8	971
50	982	51.4	980
60	987	58.4	988
70	992	66.7	994
80	997	76.0	998
90	1007	88.6	1003
100	1017	99.0	1043

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In_2Te_3-Co_3Te_4 SİSTEMİNİN FAZA DİAQRAMININ LİKVİDUS ƏYRİSİNİN TƏNLİYİ

In_2Te_3-Co_3Te_4 sisteminin hal diaqramındakı likvidus əyrisinin nəzəri qurulması üçün riyazi tənlik müəyyənləşdirilmişdir. Bu məqsədlə, iki hissədən ibarət olan likvidus əyrisini parabolanın qolları kimi qəbul edərək, parabola təni kimi qəbul edərək, parabola tənliklərindən istifadə edilmişdir. Müəyyənləşdirilən tənlikdən istifadə edərək yüksək dəqiqliklə geniş konsentrasiya intervalında qarşılıqlı təsirdə olan komponentlərin tərkiblərinin və temperaturlarının qiymətlərini hesablamaq olar. Göstərilmişdir ki, işlənmiş bu tənliyin həlli ilə müəyyən temperatur intervalında maddənin halının dəyişməsini səciyyələndirmək mümkündür.

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УРАВНЕНИЕ ЛИНИИ ЛИКВИДУСА ФАЗОВОЙ ДИАГРАММЫ СИСТЕМЫ In_2Te_3-Co_3Te_4

Установлено уравнение для расчета линии ликвидуса диаграммы состояния системы In_2Te_3-Co_3Te_4. С этой целью, линия ликвидуса, состоящая из двух ветвей, была принята подобной ветвям двух парабол, отчего и для вывода математического выражения использованы уравнения параболы. Используя предложенное уравнение можно с высокой точностью рассчитать значения состава и температуры плавления взаимодействующих компонентов в широком концентрационном интервале.

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