# THE MATHEMATICAL MODELING OF COMPONENTS DISTRIBUTION IN SOLID SOLUTIONS InSb-InAs AT THE ZONE RECRYSTALLIZATION

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The mathematical modeling of components distribution in crystals of solid solutions InSb-InAs at the zone recrystallization of the material was constructed, regarding changes of component segregation coefficient with the melt content. Concentration components profiles along ingots for various values of operation parameters (compound of the melted band) were calculated. Obtained results determine the optimal mode of InSb-InAs crystals growth with the fixed homogenous and variable contents.

The significance of the study of semiconductive solid solutions of binary systems is determined by the control possibility of fundamental crystal parameters, determined optic-electron properties of the material by means of the components ration change. It is known, that the diamond-like system of solid solutions InSb-InAs refers to the rank (class) of perspective material both in scientific and applied aspects. Results of theoretical calculations of the components distribution in this system at crystals growth from the melt by Chohralskiy method were represented in paper [1]. Analogous problems were solved recently for the system Ge-Si [2-4], results of which are in agreement with experimental data. The mathematical modeling of components distribution in quasi-binary system of solid solutions InSb-InAs at the zone recrystallization of the material was constructed in the present paper, regarding the complex nature of the change of component distribution coefficient with the melt compound. The purpose of the paper is determination of optimal operation parameters for InSb-InAs crystals preparation with fixed homogenous and variable compound.

The problem was solved in the following approximation [2,5]: the evaporation and compound components resolution (decay) are absent in the melt, InSb and InAs diffusion rates are rather high in the melt and provide the compound uniformity on the overall volume, the components diffusion in the solid phases is negligibly low, the equilibrium between liquid and solid phases, determined by the state diagram of the quasi-binary system, exists in the crystallization front, the crystallization front is plane, the compound of the original polycrystalline ingot is macroscopic homogenous.

Let us introduce following notations: $V_m^0$ and $V_m$ are volumes of the melted zone at initial and current moments: $C_c$, $C_i$, $C_m$ are molecules concentrations of the second component (InAs) in the crystal, original ingot and melt, respectively, $C_m^0$ is concentration of the second component in the melted and at the initial moment, $C$ is the total number of InAs in the melt, $V_c$ is melt volume crystallized in the time unit, $V_i$ is InSb-InAs ingot volume melted in the time unit, $K=C_0/C_m$ is equilibrium segregation coefficient InAs, $L$, and $Z$ are lengths of original ingot, melted zone and recrystallized part of the ingot, respectively.

According to the problem, conditions we consider, that the rate of the melt crystallization $V_c$ does not depend on the time and then we receive in accepted above notations:

$$C_m = \frac{C}{V_m}; \qquad \frac{\dot{C}V_m - \dot{V}_m C}{V_m^2}, \tag{1}$$

$$V_m = V_m^0 - (V_c - V_i)t \tag{2}$$

We consider, that till the final melted zone both $V_c$-$V_i$ and $V_c$ do not depend on time. In this case following relationships are right at the initial part of the ingot of the length $L$- :

$$V_m = V_m^0, \quad C_m^0 = C_i \text{ and } \dot{C} = V_c C_m K + V_i C_m^0 \tag{3}$$

Substituting (3) in (1) and dividing variables we receive after integration:

$$\int_{C_m^0}^{C_m} \frac{dC_m}{C_m^0 - C_m K} = \frac{V_c}{V_m^0} = \frac{Z}{l} \tag{4}$$

In limits of the latter melted

$$V_m = \mathrm{V_m^0} - \mathrm{V_c}t, \; \dot{V}_m = -V_c, \quad \dot{C} = -V_c C_m K \tag{5}$$

Substituting (5) in (1) after integration we receive:

$$\int_{C_{mf}^0}^{C_m} \frac{dC_m}{C_{mf}^0 - C_m k} = \ln \frac{V_m^0}{V_m^0 - V_c t}, \tag{6}$$

here $C_{mf}^0$ is the start concentration of the second component in the latter melted zone. Marking the part of the super-crystalline melt $V_c t / V_m^0$ by the symbol $g$, we rewrite the equation (6) in the following form:

$$g = 1 - \exp\left[ - \int_{C_m}^{C_{mf}^0} \frac{dC_m}{C_m K - C_m} \right] \tag{7}$$

To calculate the integrals (4) and (7) we should know the analytic dependence of the segregation coefficient $K$ on the melt compound $C_m$. For the examined system InSb-InAs versus the compound, $K$ changes in a complex way from ~20.5 to1 and does not yield to the mathematical description. The dependence diagram of $K$ on $C_m$ in the overall range of component concentration was constructed in paper [1] on the base of state diagram data of this system in conjugated solid and liquid phases. Applying these data, integrals in equation (4) and (7) may be calculated by the numerical (graphic) method [2,5].

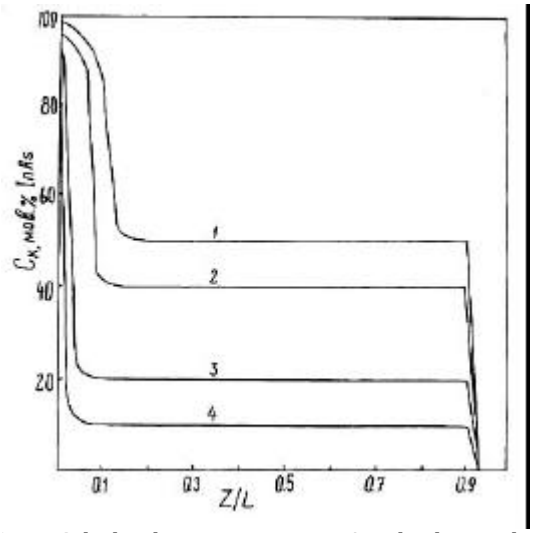


*Fig.1.* Calculated concentrations InAs alond crystals InSb-InAs, grown by the method of the zone melting. The length of the melted zone =*L/10*. The original compound of ingots is: 1 – $C_i$=*50;* 2 – *40;* 3 – *20;* 4 – *10 mole%* InAs..

The components distribution in the ingot InSb-InAS, calculated from equations (4) and (7) by the numerical method, for four various values $C_i$ is demonstrated on fig.1. In the calculation it was accepted, that =*L/10*. As it is seen from fig. 1, at all cases the concentration InAs is maximal in the ingot origin and, then, reducing, reaches homogeneity with $C_c=C_i$, At the ingot end the second component concentration again begins to fall and reaches practically zero at $Z=L$. The length of the final part with the variable compound for all examined ingots compositions, is equal to the width of the melted zone . The extent of the original part with the variable compound depends on the initial ingot composition. It is connected with the segregation coefficient change with the melted zone compound. The rate of the compound change along the crystallization direction on the final part of the melted zone falls with $C_i$ reduction, since the length of this zone is fixed according to the problem condition.

The control possibility of InAs concentration profile in the ingot by the change of the melted zone length is demonstrated on fig.1. As, for example, the distribution of InAs along the ingot InSb-InAs for four various values of is illustrated on fig.2. The original compound of all ingots is identical and contains 40 mole %.

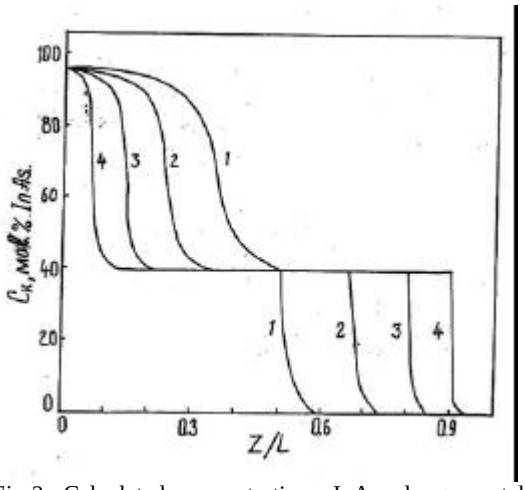


*Fig.2.* Calculated concentrations InAs along crystals InSb-InAs, grown by the method of the zone melting from the original compound $InSb_{0.6}InAs_{0.4}$. The length of the melted zone is: 1 – =*L/2;* 2 –*L/3;* 3 –*L/5;* 4 –*L/10*..

The influence efficiency of operation parameters on the components redistribution in the ingot InSb-InAs at the zone recrystallizat ion of the material is visually demonstrated on curves of fig.2.

As it is seen, the length of the melted zone in wide (broad) limits determines the extent of crystals parts with variable and homogenous compounds.

Family of curves of fig.1 and 2 shows the possibility of mathematical modeling for operation parameters determination and optimal technological conditions for InSb-InAs crystals growth with the fixed homogenous or variable compounds.

The following conclusion may be done on the base of aforesaid data and results.

The mathematical modeling of component distribution in solid solutions InSb-InAs, at the zone recrystallization of the material, conducted, regarding the dependence of components segregation coefficient with the melt compound, allows to value optimal technological parameters, as the original compound of the ingot and length of the melted band, with the purpose of the crystals receipt with the fixed components distribution.

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