THE INFLUENCE OF MOLTEN ZONE LENGTH ON COMPONENT DISTRIBUTION AT ZONE RECRYSTALLIZATION OF InSb-GaSb SOLID SOLUTIONS

G.H AJDAROV, M.A. AKPEROV, A.I. ALEKPEROV, Z.A. AGAMALIYEV
G.B. Abdullayev Institute of Physics of Azerbaijan National Academy of Sciences
AZ-1143, H. Javid ave., 33, Baku, Azerbaijan

It is shown that by mathematical modeling the component concentration profile can be controlled in wide limits at zone recrystallization of InSb-GaSb solid solutions by the way of change of the molten zone length. It is seen that the obtained results define the optimal technological parameters (molten zone length, ingot initial composition) for growing of InSb-GaSb crystals with given homogeneous and variable compositions.

The solid solutions of InSb and GaSb semiconductor compounds are related to perspective materials in both scientific and applied aspects. The detail investigations of phase state diagram show that the composite components of this system totally dissolve in each other in any proportion [1]. This circumstance gives the possibility to manipulate by semiconductor fundamental parameter value by means of simple change of matrix composition. The zone melting is the one of effective and simple crystal growing methods of solid solutions with given homogeneous and variable compositions.

In the present paper the mathematic modeling of molten zone length influence on component distribution character in single crystals of InSb-GaSb solid solutions at zone recrystallization of initial melt has been carried out. The aim is the method possibility establishment of zone recrystallization and optimal operational parameters for crystal growing with given variable and constant compositions. The analogous tasks in Pfann approximation have been solved in works [2-7] for crystals of silicon – germanium system grown by both conservative and non-conservative methods. The results of these works show the well agreement with experimental data carried out in this direction.

The mathematical task of component distribution in InSb-GaSb crystal grown by traditional method of zone melting has been solved at the fulfillment of standard conditions [8]: the diffusion rates of InSb and GaSb molecules in molten zone are enough high ones and provide the composition uniformity on its whole volume; the diffusion of components in solid phase is neglible one during growth; the equilibration between liquid and solid phases defined by state diagram exists on crystallization front; the segregation component coefficients change with melt composition in the correspondence with phase state diagram of InSb-GaSb system; the evaporation and decomposition of composite components are absent in melt; the crystallization front is plane one; the composition of initial polycrystalline ingot is macroscopically homogenous one.

Let's introduce the following designations: L, l, and Z are lengths of initial ingot, ingot recrystallized part and molten zone correspondingly; V_m^0 and V_m are volumes of molten zone in initial and current moments; C_c, C_i, C_m are molecule concentrations (shares) of second component (GaSb) in the crystal, initial ingot and melt correspondingly; C_m^0 is second component concentration in molten zone in initial moment; C is total GaSb in the melt; V_c is melt volume crystallizing in time unit; V_i is InSb-GaSb ingot volume melting in time unit; $K=C_c/C_m$ is segregation equilibrium, V_c is melt volume crystallizing in time unit; V_i is InSb-GaSb ingot volume melting in time unit; $K=C_c/C_m$ is GaSb segregation equilibrium coefficient.

In accepted designations under the condition of melt crystallization constant rate we have the following formulas:

$$C_m=\frac{C}{V_m};\quad \frac{dC_m}{dt}=\frac{\dot{C}V_m-\dot{V}_mC}{V_m^2};V_m=V_m^0-(V_c-V_i)t \qquad (1)$$

Z and V_i, V_c don't depend on time up to final molten zone. Then on ingot part of L-Z length in crystallization process are true the following relations:

$$V_m=V_m^0,\ C_m^0=C_i \text{ and } \dot{C}=V_cC_m\,K+V_iC_m^0 \qquad (2)$$

Substituting (2) into (1), after series of transformations and integration we have:

$$\int_{C_m^0}^{C_m}\frac{dC_m}{C_m^0-C_mK}=\frac{l}{Z} \qquad (3)$$

The equation (3) find the crystal composition by its ℓ length on the section from origin of one up to L-Z.

From the time moment of final molten zone formation of Z length we have:

$$V_m=\mathrm{V_m^0}-\mathrm{V_c}t,\ \dot{V}_m=-V_c,\ \dot{C}=-V_c\,C_mK \qquad (4)$$

Substituting the data (4) into (1) after integration we obtain:

$$\int_{C_{mf}^0}^{C_m}\frac{dC_m}{C_{mf}^0-C_mk}=\ln\frac{V_m^0}{V_m^0-V_ct} \qquad (5)$$

Here C_{mf}^0 is second component concentration in final molten zone in the time moment of its formation. Designating the part V_ct/V_m^0 of crystallized final zone by γ symbol, let's write the equation (5) in the following form:

$$\gamma = 1 - \exp\left[- \int_{C_m}^{C_{mf}^0} \frac{dC_m}{C_m K - C_m} \right] \qquad (6)$$

For the solving of integrals in equation (3) and (6) we need the knowing of analytic dependence K on C_m. The dependence of K on C_m calculated from phase diagram data of GaSb-InSb system [1] is shown on fig.1. As it is seen from fig.1 K changes very complicated with melt composition in wide range from value ~ 10,5 up to 1 and doesn't obey to analytical description. However, data of fig.1 allow us to define the integral values in equations (3) and (6) by numerical method [2,5]. As each value of melt composition corresponds to conjugated value $C_c=C_lK$, one can construct the dependence plot of component concentration distribution on crystal length.

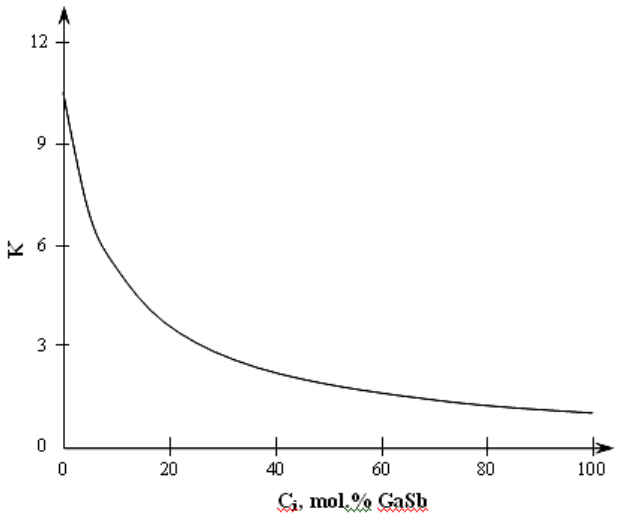

Fig.1. The dependence of segregation coefficient GaSb (K) on GaSb-InSb melt composition calculated on data of phase state diagram [1].

The character curves of component concentration distribution in InSb-GaSb ingots calculated from equations (4) and (7) by numerical method for four different Z values are shown on fig.2. The initial composition of all ingots is similar and consists in 20 mol%GaSb. The fig. 2 visually demonstrates the essential influence of operation parameter Z on component redistribution in InSb-GaSb ingot at zone recrystallization. As it is seen the both lengths the homogeneous and heterogeneous crystal parts on the composition are defined by molten zone width. The family of curves on the fig.2 shows that the possibilities of mathematical modeling for definition of optimal operational parameters for growing of InSb-GaSb crystals with given homogeneous and variable compositions.

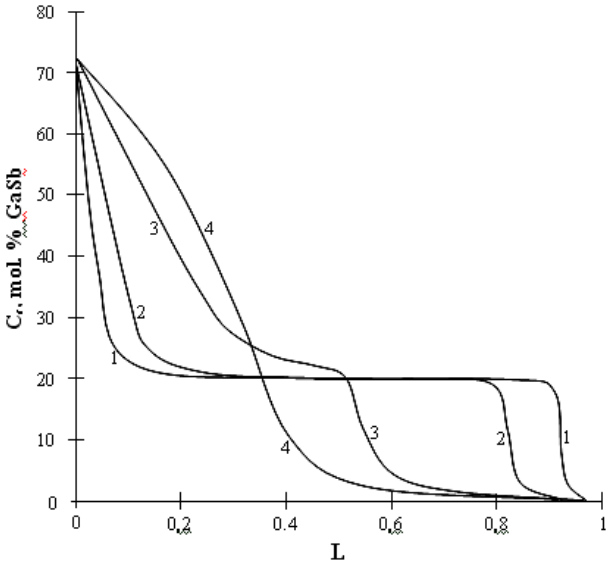

Fig.2. The concentrational profile GaSb in InSb-GaSb solid so lution crystals grown by zone melting method from $In_{0.8}Ga_{0.2}Sb$ initial ingot. The molten zone length: (1) – $Z=L/10$, (2) – $Z=L/5$, (3) – $Z=L/2$, (4) – $Z=L$. L is initial ingot length.

We can make the following conclusion on the base of above mentioned data and results. The mathematical modeling of component distribution in InSb-GaSb crystals grown by zone melting method carried out taking under consideration the complex dependence of component segregation coefficients on the melt composition allows us to estimate the optimal technological parameters such as molten zone length and ingot initial composition for crystal obtaining with given composition and component distribution.

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H.X. Əjdərov, M.A. Əkbərov, A.İ. Ələkbərov, Z.A. Ağamalıyev

ZONA KRİSTALLAŞMASI ZAMANI InSb-GaSb BƏRK MƏHLULLARINDA KOMPONENTLƏRİN PAYLANMASINA ƏRİNTİ ZOLAĞININ UZUNLUĞUNUN TƏSİRİ

Riyazi modelləşdirmə əsasında göstərilib ki, ərinti zolaq üsulu ilə alınan InSb-GaSb kristallarında komponentlərin konsetrasiyon profili ərinti zolağın uzunluğunun dəyişməsi ilə geniş intervalda idarə edilə bilər.Göstərilib ki, alınan nəticələr verilmiş bircinsli və dəyişən tərkibli InSb -GaSb kristalları əldə etmək üçün optimal texnoloji parametrləri (ərinti zolağın uzunluğu, ilkin bərk məhlulun tərkibi) müəyyən edilir.

Г.Х Аждаров, М.А. Акперов, А.И. Алекперов, З.А. Агамалиев

ВЛИЯНИЕ ДЛИНЫ ЗОНЫ РАСПЛАВА НА РАСПРЕДЕЛЕНИЕ КОМПОНЕНТОВ ПРИ ЗОННОЙ ПЕРЕКРИСТАЛЛИЗАЦИИ ТВЁРДЫХ РАСТВОРОВ InSb-GaSb

Математическим моделированием показана возможность управления в широких пределах концентрационным профилем компонентов при зонной перекристаллизации твёрдых растворов InSb-GaSb путём изменения длины расплавленной зоны. Показано, что полученные результаты определяют оптимальные технологические параметры (длина расплавленной зоны, стартовый состав слитка) для выращивания кристаллов InSb-GaSb с заданным однородным и переменным составами.

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