MODELLING OF COMPONENT AXIAL CONCENTRATION PROFILES IN InSb-GaSb SOLID SOLUTION SINGLE CRYSTALS GROWN BY ZONE MELTING METHOD USING InSb AND GaSb SEEDS

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The problem of component concentration distribution in InSb-GaSb solid solution crystals grown by zone melting method using InSb and GaSb seeds is solved in Phann approximation. The component axial concentration profiles in crystals grown in initial macro-homogeneous ingots InSb-GaSb with different composition are calculated taking under consideration the complex change of GaAs segregation coefficient with molten zone composition. It is shown that results obtained by mathematical modeling define the possibilities of zone melting modified method and optimal conditions for growth of InSb-GaSb crystals with given homogeneous and alternative compositions.

Keywords: InSb, GaSb, solid solutions, Phann approximation, segregation, molten zone, component distribution.
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INTRODUCTION

The material obtaining with given component axial concentration profile and also the supply of its monocrystallinity are the main tasks of growth process of semiconductor solid solution bulk crystals from melt.

InSb-GaSb system takes the special interest in wide range of semiconductor solid solutions. The component composite of this system is widely used in modern micro- and opto-electronic industry. Besides, InSb and GaSb totally solving in each other in any ratios in both liquid and solid states and form the continuous series of exchange solid solutions [1].

The math task by definition of component distribution along InSb-GaSb solid solution single crystals grown by zone melting modified method with use of seeds from InSb and GaSb is solved in present work in Phann approximation. The aim is the establishment of possibilities of zone melting method for InSb-GaSb single crystal growth with given homogeneous and alternative compositions. The tasks by concentration profile modeling of such type had been solved earlier for Ge-Si crystals and series of semiconductor compounds of A3-B5 type grown up from the melt by different conservative and non-conservative methods [2-9]. The results of these works show the well agreement of the theory with experiment.

The conceptual scheme of InSb-GaSb single crystal growth by zone melting modified method put in the base of math solution of the given task is presented in fig.1. The monocrystalline seed (1) from InSb or GaSb (fig.1A) is put in the low part of cylindrical type crucible. The priori prepared crucibles from InSb (2) and macro-homogeneous solution InSb-GaSb with the given composition are put under the seed. The crucible melting (2) from InSb positioned directly under the seed (fig.1 B) is carried out in vacuum condition. The temperature in boundaries of the melt with the seed and ingot at the moment of recrystallization beginning is equal to InSb melting temperature. The crystal growth takes place on the seed with from the moment of switching mechanism of crucible shift relatively the heater and continues up to total ingot recrystallization.

The task of axial component concentration distribution along InSb-GaSb crystal grown in above mentioned conditions is solved in Phann approximation at which the following conditions are carried out [10]: diffusion rates of InSb and GaSb components in the melt are enough high ones and cause its homogeneity in whole volume; component diffusion in solid phase is negligible one; crystallization front is plane one; there is the equilibrium between liquid and solid phases in crystallization front; GaSb segregation coefficient changes in dependence on the melt composition in the correspondence with phase state equilibrium diagram of InSb-GaSb system; thermal expansion or compression of the material at phase transitions is negligible; the composition of initial polycrystalline ingot InSb-GaSb is macro-homogeneous one.

THEORETICAL CALCULATIONS

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

Following expressions in these designations are:

$$C_m = \frac{C}{V_m}; \quad \frac{dC_m}{dt} = \frac{\dot{C}V_m - \dot{V}_m C}{V_m^2} \quad \text{and}$$

$$V_m = V_m^0 - (V_c - V_i)t \quad (1)$$

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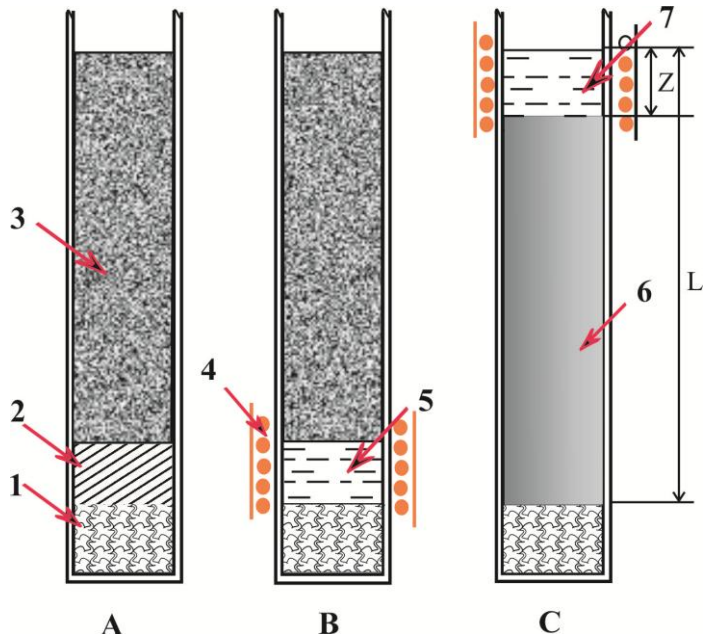

Fig.1. The conceptual scheme of InSb-GaSb solid solution single crystals growth by zone melting modified method. A is order of crucible loading; 1, 2 are seed and rod from InSb; 3 is macro-homogeneous rod of InSb-GaSb given composition; B is crystallization starting point; 4 is heater; 5 is melt from InSb; C is moment of final molten zone formation; 6 is InSb-GaSb single crystal; 7 is InSb-GaSb melt; L and Z are lengths of given regions.

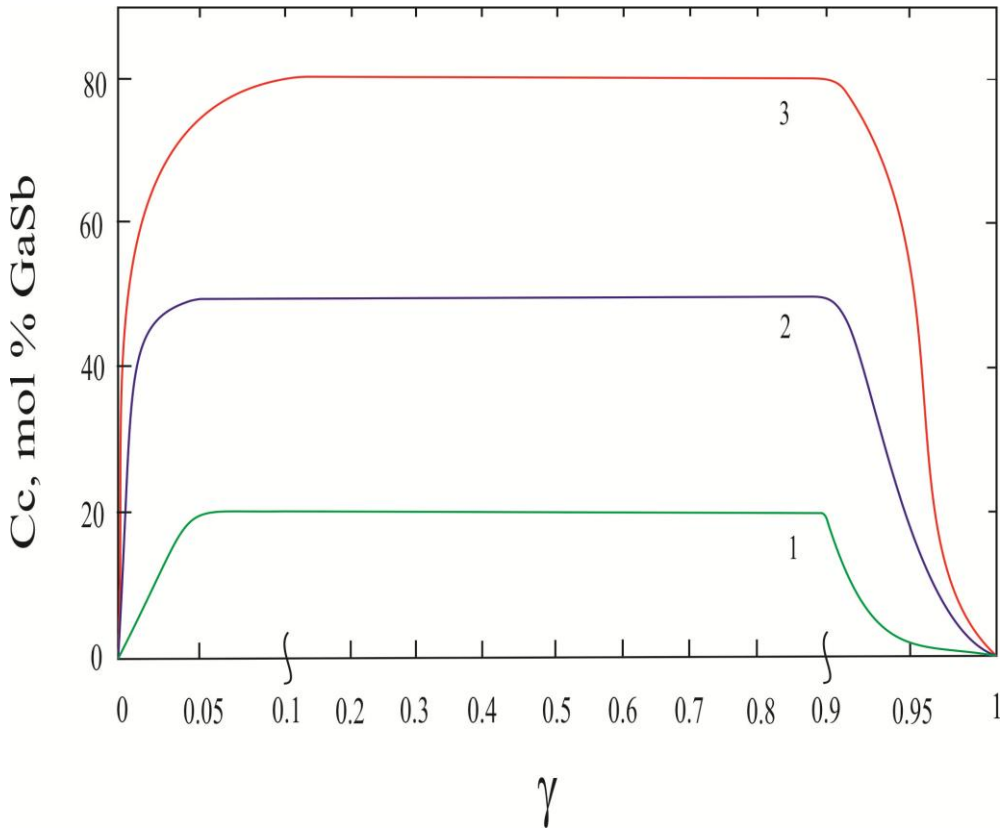

Fig.2. The calculative axial concentration profiles GaSb in InSb-GaSb single crystals grown by zone melting method. The molten zone length is Z=0.1 L. The composition of initial macro-homogeneous ingots InSb-GaSb: 1 – 20, 2 – 50, 3 – 80 at.% GaAs.

By task condition we consider that the melt recrystallization rate (V_c) doesn't depend on time in process of whole technological cycle and Z and V_i parameter values stay unchangeable ones up to the moment of final molten zone formation. In this case the following equations are equal in region of crucible with L-Z length from the seed (fig.1):

$$V_m = V_m^0 \; ; \quad C_m^0 = 0; \quad V_i = V_c \qquad \text{and}$$

$$\dot{C} = V_i C_i - V_c C_m K \qquad (2)$$

Taking under consideration (2) from equations (1) we have the division of alternatives and integration after series of transformations:

$$\int_0^{C_m} \frac{dC_m}{C_i - C_m K} = \frac{V_c t}{V_m^0} = \frac{l}{Z} \qquad (3)$$

We have from the moment of final molten zone formation of Z length:

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

Taking under consideration (4) we obtain after series of transformations and integration:

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

Here C_{mf}^0 is initial concentration part of GaSb in the melt in moment of final molten zone formation. Let's write the equation (5) in the following form designated the length and part of melt crystallized part ($V_c t / V_m^0$) in t moment by l^* and γ symbols correspondingly:

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

The definition of l/Z and γ as C_m function is the same as $C_c = K \, C_m$ along whole material length treated by zone crystallization requires the integral solution in equations (3) and (6) in which the segregation coefficient of second component (K) depending on C_m is included. It is known that K value in InSb-GaSb system changes enough difficultly in wide limits in dependence on melt composition [1]. This circumstance leads to the necessity of calculations of integrals in (3) and (6) by numerical method by the way of $K = C_c / C_m$ conjugated values in corresponding intervals of C_m change on data of system equilibrium phase state diagram.

The character curves of GaSb concentration distribution by solid solution crystal lengths InSb-GaSb calculated from equations (3) and (6) and relation $C_c = C_m K$ are presented in fig.2. The calculations are carried out for three different values C_i (x=0.2; 0.5; 0.8) of InSb-GaSb initial ingot at molten zone length Z=0,1L. As it is seen from fig.2, GaSb concentration in initial part of all crystals increases on the length from zero up to corresponding value C_i of initial homogeneous ingot InSb-GaSb. Further, C_c value with crystal growth stays constant up to final zone formation by length Z=0.1 L. In this part of ingot GaAs concentration begins to decrease with *l* increase and tends to zero at *l*=L. The length of initial part with GaSb increasing concentration and final one with GaSb decreasing concentration is similar for all samples and is equal to molten zone length Z=0.1 L. Note that the enough strong increase of GaSb concentration in these parts of all ingots which causes the big output of solid solution single crystals with homogeneous composition is of great interest.

CONCLUSION

The curve family (fig.2) demonstrates the potential and availability of zone melting method for growing of InSb-GaSb solid solution single crystals with given homogeneous and alternative compositions. Summarizing the above mentioned one can state the following. The mathematical modeling of component axial concentration distribution along InSb-GaSb crystals grown up by zone melting method with use of seeds from InSb and GaSb allows us to estimate the optimal technological parameters for single crystal obtaining of this system with given distribution and component concentration.

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