# MODELLING OF MOLTEN ZONE LENGTH INFLUENCE ON COMPONENT CONCENTRATION DISTRIBUTION IN InAs-GaAs CRYSTALS GROWN BY MODIFIED ZONE MELTING METHOD

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The task of component concentration distribution along Ge-Si solid solution crystals grown by modified zone melting method using the InAs-seed crystal is solved in the fully mixed melt approximation.

The component axial concentration profiles in crystals grown at different molten zone lengths are calculated taking under consideration the complicated dependence of GaAs segregation coefficient on the melt composition. The possibility of control by component concentration distribution in wide range in InAs-GaAs crystals by the way of molten zone length changes is shown. The analysis of obtained results defines the optimal technological parameters for growing of solid InAs-GaAs solution crystals with given homogeneous and alternative compositions along the matrix.

**Keywords:** InAs, GaAs, solid solutions, Phann approximation, molten zone, component distribution.
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## INTRODUCTION

The obtaining of material with given concentration component distribution in matrix and support of its monocrystallinity is the main technological problem of volume crystal growing of semiconductor solid solutions from the melt.

InAs-GaAs system the composite components of which are the basic materials of modern micro-and opto-electronic industry, presents the special interest in the set of semiconductor solid solutions. In and GaAs fully dissolve in each other in any ratios in both liquid and solid states and form the continuous set of exchange solid solutions [1].

The math modeling of component concentration profile along InAs-GaAs crystals grown by modified zone recrystallization method using InAs-seed crystal is carried out in the given work in Phann approximation. The aim is potential establishing of modified method for obtaining of InAs-GaAs volume single crystals with given component axial concentration distribution. Note that the tasks on modeling of component concentration profiles are solved earlier for Ge-Si crystals grown from the melt by the series of conservative and non-conservative methods [3-10]. The results of these works show the well coincidence with experimental data.

## RESULTS AND DISCUSSIONS

The conceptual scheme of solid solution crystal growing by modified method of zone melting is presented in fig.1. The single-crystal seed (1) from InAs (fig.1A) is put into crucible of cylinder form. The previously prepared rods of definite diameter from InAs (2) and macro-homogeneous solid solution InAs-GaAs with given composition (3) are put under seed. The rod melting (2) from InAs put directly under seed (fig.1B) is carried out in vacuum conditions. The temperature in melt boundaries with seed and ingot in prestarting moment of recrystallization is equal to melting point of InAs. The crystal growth takes place in seed from the moment of switching of crucible-moving mechanism relatively to heater and continues up to ingot total recrystallization (3). The length of final molten zone is supported as constant and equal to Z up to moment of its formation. Here the final molten zone consists in pure InAs as opposed to traditional zone melting method [2,11]. This circumstance solves the problem of seed which is necessary for growing of single crystals of Ge-Si solid solutions of different compositions by the way of using the InAs-seed.

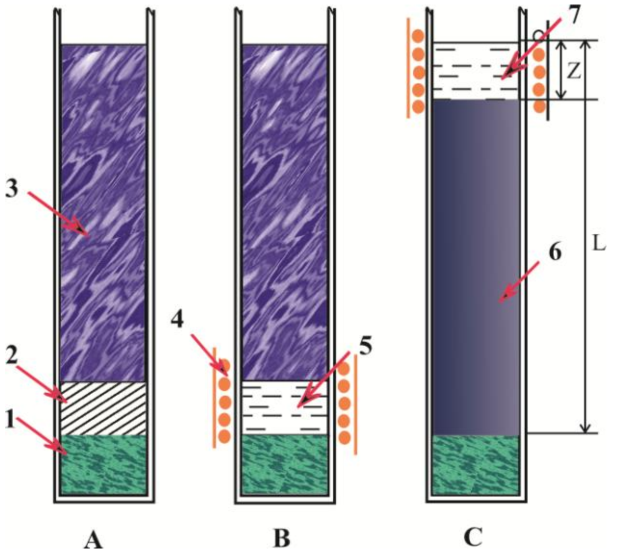

*Fig.1.* Growing circuit of single crystal InAs-GaAs solid solutions by modified zone melting method using the InAs-seed. A is order of crucible loading: 1 and 2 are seeding and rod from InS, 3 is macro-homogeneous rod from InAs-GaAs of given composition, C is moment of final molten zone formation; B is crystallization starting point: 4 is heater, 5 is melt from InAs, C is moment of final molten zone formation: 6 is InAs-GaAs single crystal, 7 is InAs-GaAs meltl L and Z are lengths of given regions.

The task of concentration distribution of InAs and GaAs along InAs-GaAs crystal grown by modified zone melting method is solved in Phann approximation at carrying out of following standard conditions [11]: component diffusion in solid phase is negligible quantity; crystallization front is plane; there is the equilibrium between liquid and solid phases in crystallization front; the diffusion rate of composite elements of InAs and GaAs in the melt supplies its homogeneity in all volume (totally mixed melt); the coefficients of component segregation of the melt change with equilibrium phase state diagram of InAs-GaAs system; thermal expansion or compression of material at phase transitions is negligible quantity; the composition of InAs-GaAs initial ingot is macro-homogeneous one.

Let's introduce the following designations: $C_c$ , $C_i$ , $C_m$ are concentration parts of GaAs second component in crystal, initial polycrystalline rod and melt correspondingly; $C$ is general concentration part of GaAs atoms in melt; $C_m^0$ is concentration part of GaAs in molten zone in initil time; $V_c$ is melt volume crystallizing in time unit; $V_i$ is volume of initial ingot InAs-GaAs, melting in time unit; $V_m^0$ and $V_m$ are volumes of molten zone in initial and current time; $K = C_c / C_m$ is segregation equilibrium coefficient GaAs; L is general length of initial rods from InAs and InAs-GaAs; $\ell$ is length of recrystallized part of material in t moment; Z is molten zone length.

We have in limits of accepted designations:

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

$$V_m = V_m^0 - (V_c - V_i)t \; ; \tag{1}$$

By statement of a problem Z , $V_i$ and $V_c$ parameters don't depend on time up to the formation of final molten zone. In this case the following ratios are carried out in region by L-Z length from seed (see fig.1A and fig.1C

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

$$\dot{C} = V_i C_i - V_c C_m K \tag{2}$$

Substituting (2) in (1) after set of transformations and integration we have:

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

Taking under consideration the equality $K = C_c / C_m$ the equation (3) defines the component by the length of growing crystal in region from $\ell$ =0 up to $\ell$ = L-Z .

The following ratios are carried out in final region from moment of molten zone formation by Z length:

$$V_i = 0 , \quad V_m = \mathrm{V_m^0} - \mathrm{V_c} t \; , \quad \dot{V}_m = -V_c \; ,$$
$$\dot{C} = -V_c \, C_m K \tag{4}$$

We have the following after series of transformations and integrations from equation (1) taking under consideration (4):

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

Here $C_{mf}^0$ is start concentration part of GaAs atoms in the melt in moment of final molten zone. Designating the length and crystallization part of the final zone melt ( $V_c t / V_m^0$ ) in t moment by $l^*$ and $\gamma$ symbols correspondingly, let's write the equation (5) in following form:

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

The definitions of $l/Z$ and $\gamma$ as $C_m$ function (as $C_c = K \, C_m$) along whole material length treated by zone recrystallization, requires the integral solution in equations(3) and (6). The segregation coefficient of second component (k) including in both these equations depends on $C_m$ [1]. This circumstance leads to necessity of integral calculation in (3) and (6) by numerical method with use of data of phase equilibrium state diagram of InAs-GaAs. Give gradually $C_m$ values in required interval and define the K values conjugated with it, the integrals in (3) and (6) are solved by numerical method.

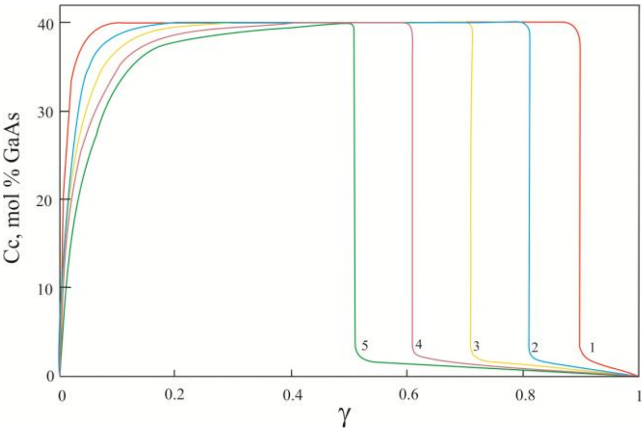

*Fig.2.* The calculative concentration profiles of GaAs along InAs-GaAs single crystals grown by modified zone melting method at different values of molten zone length Z. 1,2,3,4 curves correspond to values Z/L = 0,1, 0,2, 0,3, 0,4, 0,5 correspondingly. The composition for all initial ingots of solid solutions is equal to $\mathrm{InAs_{0.6}}$-$\mathrm{GaAs_{0.4}}$.

The character curves of GaAs concentration distribution along crystals InAs-GaAs for different Z values calculated from equations (3) and (6) taking under consideration ratios $C_c = C_m K$ are presented in fig.2. In calculations the start composition of all initial macro-homogeneous rods is equal to $InAs_{0.6}$-$GaAs_{0.4}$.

As it is seen from this figure Z operational parameter significantly influences on component redistribution at zone recrystallization of InAs-GaAs initial rod of the given composition. Moreover, the lengths of both homogeneous and heterogeneous crystal parts by composition are defined by molten zone value Z. The curve family (fig.2) directly demonstrates the potential and availability of modified method of zone melting for obtaining of solid solution single crystals InAs-GaAs with required homogeneous and alternative compositions by the way of choice of corresponding values of technological parameters (Z, $C_i$).

## CONCLUSION

Summarizing the above mentioned one can conclude the following. The math modeling of component axial distribution in crystals InAs-GaAs grown by modified method of zone recrystallization and carried out taking under the consideration the complex character of component segregation coefficient change with melt composition gives the possibility to evaluate the optimal technological parameters (molten zone length and initial composition of feeding rod) for obtaining of solid solution crystals with given component concentration profile.

[1] *V.S. Zemskov, V.B. Lazarev*. Tverdie rastvori v poluprovodnikovix sistemax. «Nauka», Moskva, (1978) 197. (In Russian).

[2] *J. Schilz, V.N. Romanenko.* Bulk growth of Silicon-Germanium Solid Solutions, J. Materials in Electronics,V.6 (1995) 265-279.

[3] *G.Kh. Azhdarov, T. Kucukomeroglu, A. Varilci et al.* Distribution of components in Ge-Si bulk single crystals grown under continuous feeding of the melt with the second component (Si), J. Crystal Growth, 226 (2001) 437-442.

[4] *I. Kostylev, J.K. Woodacre, Y.P. Lee et al.* Melt zone growth of Ge-rich Ge1-xSix bulk single crystals, J. Crystal Growth, 377 (2013)147-157.

[5] *T.A. Campbell, M. Schweizer, P.Dold et al.* Float zone growth and characterization of Ge1-xSix (x<10 at%)single crystals, J. Crystal Growth, 226 (2001) 231-237.

[6] *N.V. Abrosimov, S.N. Rossolenko, W. Thieme et al.* Czochralski growth of Si- and Ge-rich SiGe single crystals, J. Crystal Growth, 174 (1997) 182-186.

[7] *Z.M. Zakhrabekova.* Kristalli tverdix rastКристаллы твёрдых растворов Ge-Si. Poluchenie i elektricheskie svoystva slojnoleqirovannix кристаллов Ge-Si с primesyami medi, alyuminiya I surmi, LAP LAMBERT Academic Publishing, Germaniya (2013) 139. (In Russian).

[8] *V.K. Kazimova.* Kristalli Ge-Si I ix svoystva. Poluchenie I elektricheskie svoystva tverdix rastvorov Ge-Si, slojnoleqirovannix primesyami medi, indiya I surmi, LAP LAMBERT Academic Publishing, Германия (2013) 144. (In Russian).

[9] *G.Kh. Azhdarov, R.Z. Kyazimzade.* Growth of homogeneous single crystals of Ge-Si solid solutions by the modified Bridgman method, Crystallography Reports, 50 (2005) S149-S153.

[10] *G.Kh. Azhdarov, Z.M. Zeynalov, Z.A. Agamaliyev, A.I. Kyazimova.* Growth of single crystals of semiconductor solid solutions by double feeding of the melt method, Crystallography Reports, 55 (2010)763-767.

[11] *V.M. Glazov, V.S. Zemskov.* Fiziko-ximicheskie osnovi leqirovaniya poluprovodnikov. M.: Nauka, (1967) 371. (In Russian).

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