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L.S. Lunin / I.A. Sisoev / S.Ju. Gazarjan / R.P. Veliev / A.A. Barannik

Obtaining of light emitting diodes and solar cells on the basis of AlGaAs/GaAs nanostructures

FUNCTIONAL ELECTRICAL AND ELECTRONIC MATERIALS AND DEVICES

Nowadays a large-scale search is carried out to obtain ultra-sensitive photodiodes and high-performance solar cells on the basis of AlGaAs/GaAs nanostructures. This work investigates the peculiarities of multiple recrystallization of TGZR process (Temperature Gradient Zone Recrystallization), which lets us generate nanostructures provided there is a component with big distribution coefficient. The objective of this research is to determine conditions, in which nanostructures of electronic technology can be generated through TGZR method on the basis of AlGaAs/GaAs heterostructures.

To obtain nanostructures we generally use molecular beam epitaxy (MBE), metallo-organics vapor-phase epitaxy (MOVPE), more seldom do we use liquid phase epitaxy (LPE). The given paper examines the ways of applying one of the variants of LPE, particularly TGZR method, to obtain nanostructures. Technical equipment necessary for TGZR is constituted by two flat heating units, which are placed against each other at a distance no more than 10 mm. There is a so-called “sandwich”, which consists of two semiconductor substrates (plates), and liquid zone between them. There is also a production carrier between the heaters, in which we create axial temperature gradient ranging from 0 to 100 Grad/sm under the temperature of 850ºC. Numerical modeling methods help to describe physical processes, on which the described technology is based. These methods facilitate investigation of growth kinetics of low-dimensional epitaxial layers, voltage distribution at the atomic level as well as modeling processes of growing low-dimensional epitaxial structures on technological complexes. While modeling the process of crystallization of A3B5 compounds it was determined that nanostructures can be obtained only if there is a component with high segregation index ($K>50$) and small values of liquid zone thickness ($L<20$ mcm) under multiple recrystallization.

Modeling of TGZR process is based on empirically revealed calculation dependencies of crystallization velocity for three, four, five components solid solution of the compounds A3B5 on the GaAs base. Solid solution composition and physical parameters of its epitaxial layers are calculated through generally accepted formulae. On the basis of experimental data the author determined the dependence of epitaxial layer growth velocity on the thickness of liquid zone and solid solution composition with temperature range from 700 to 1000ºC:

$$V_K = F \cdot B^{X_S P} \cdot L \cdot C^{X_S Al} \cdot e^{D \cdot E^{X_S In} \cdot L} \cdot e^{\frac{25000}{R \cdot T}}$$

where L – liquid zone thickness in mcm;

A, B, C, D, E – some constant values:

A=2, B=0, C=0,001, D=-0,006, E=0,5, F=58, R – universal gas constant; T – temperature, measured in ºC;

X_sP, X_sAl, X_sIn – concentration of phosphor, aluminum, indium in solid phase;

V_k – growth speed in mkm/hour.

Solving a system of equations to determine concentration in solid phase:

$$\begin{cases} X_sAl = X_lAl * K_{Al} \\ X_sGa = X_lGa * K_{Ga} \\ X_sIn = X_lIn * K_{In} \\ X_sP = X_lP * K_P \\ X_sAs = X_lAs * K_{As} \end{cases}$$

we should take into account the fact, that during TGZR process concentration of components in liquid phase is constantly changing in accordance with conditions of crystallization and presence of some component in a source. I-component concentration in liquid phase can be found from the following equation:

$$\frac{dX_{li}}{dh} = -\frac{K_i X_{li} - X_{s0i}}{L}$$

in which Xli – concentration of i-component in liquid phase;

K_i – distribution component of i-component

X_{s0i} – concentration of i-component in a source;

L – liquid zone thickness;

h – thickness of formed layer. dh value can be calculated through the following equation:

$$dh = dt \cdot V_{кр}$$

On the basis of above-mentioned facts we worked out a program model of TGZR process, which permits to dynamically preset parameters and apply given real processes. The program is developed with regard to empirically stated regularities in growth of structures A3B5 and implies calculation of physical parameters of generated layers.

Real technological processes can be predicted with the program of crystallization process modeling, which was developed in light of thermodynamics of multicomponent solid solutions A3B5 and parameters, calculated on the basis of trial experiments.

The results of modeling realized on developed software help to determine peculiarities of crystal formation with repeated interchange of direct and reverse crystallization processes by change of gradient direction. It was stated that extra-fine elastically strained layers of solid solutions are generated near the surface of target base at the moment, when thermodynamic balance shifts from solution to crystallization.

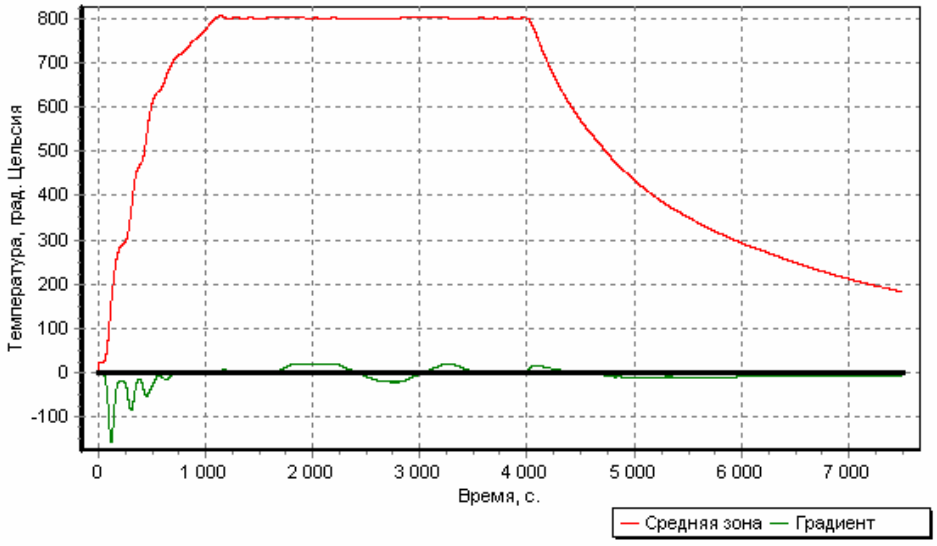


Fig.1 Time-temperature duty of the real TGZR process, maintained by digital software control complex ATSTEK-10

In the process of modeling, it was revealed that the crystallization process of obtaining nanostructures by TGZR is characterized by high sensitivity to small temperature changes in liquid zone, when the direction of temperature gradient changes. Technical software complex of technological process control was

developed to maintain the prescribed temperature with high accuracy (≤ 0,05 K); this complex helped to create the necessary conditions, which are necessary for the process of nanostructure formation by TGZR. Figure 1 shows the real time-temperature duty of TGZR; it can be seen that the temperature in the middle zone (red line) is almost constant within the range from 1200 to 4000 sec., even when the direction of temperature gradient changes (green line).

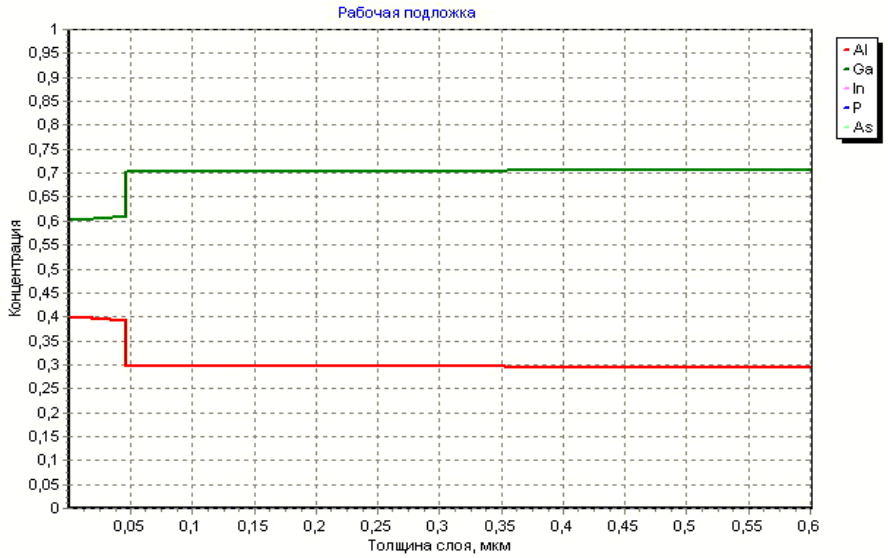
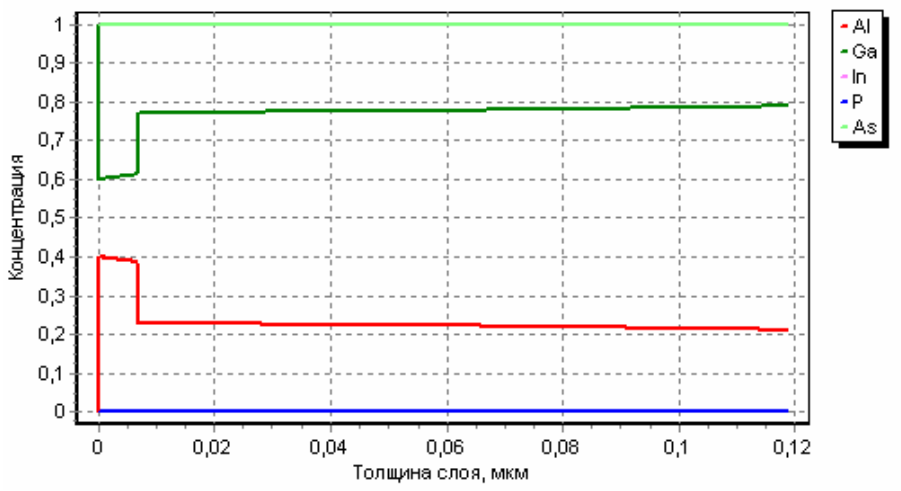


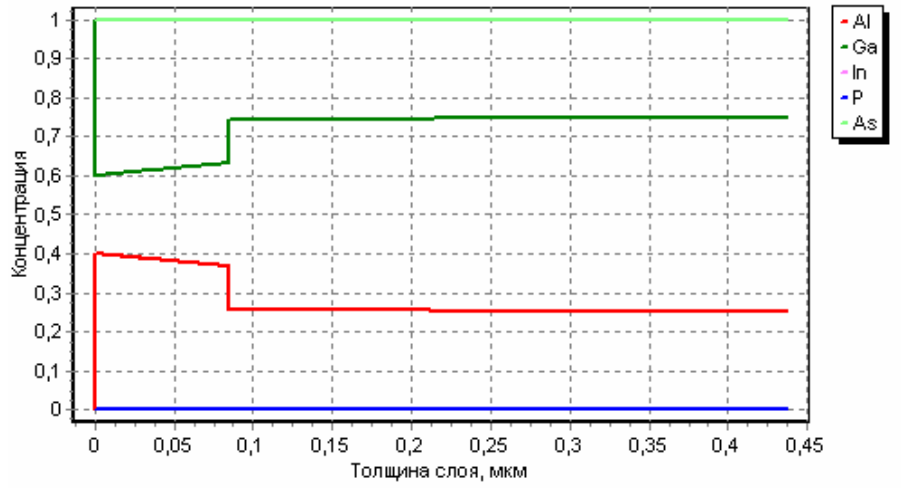
Fig. 2. Calculation correlation of component distribution in solid solution $Al_xGa_{1-x}As$ with regard to the data of time-temperature duty of TGZR, realized in a trial experiment (see Fig. 1)

The second characteristic of the developed technical software device is the possibility to use real data of TGZR temperature regime in order to calculate physical properties and compare it with ideal calculations. This helps us to make a certain forecast about the possibility of qualitative nanostructures formation under real temperature regime of TGZR (Fig. 2).

The third characteristic of the developed method is the influence of distribution coefficient of highly segregating component on the thickness of liquid zone which is regulated to provide the necessary balance of layer composition (Fig. 3).



a)



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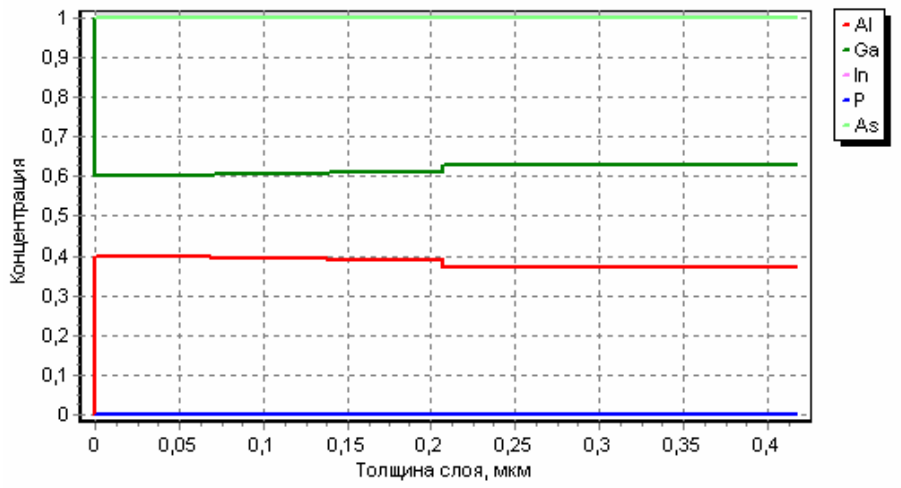

c)

Fig. 3 Calculation distribution of components in solid solution $Al_xGa_{1-x}As$, provided that the liquid zone has different thickness: a) L=10 mcm, b) L=20 mcm, c) L=50 mcm

Regularities, analyzed in a given paper, help to obtain nanostructures of A3B5 compounds given there is a component with distribution coefficient no less than 50 and thickness of liquid zone no more than 50 mcm.

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