SIMULATION OF THE DIFFUSION OF SILICON IN GALLIUM ARSENIDE.
4. DPSU PROGRAM AND RESULTS OF NUMERICAL CALCULATIONS

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A program is developed for simulating the diffusion of silicon in gallium arsenide, and numerical calculations are performed for the process of high-concentration doping of gallium arsenide during thermal diffusion of silicon from a source with a constant concentration of the impurity near the surface of the semiconductor.

4.1. DPSU Program. A proposed model of diffusion processes in composite semiconductors [1, 2] and a numerical method for solving the diffusion equation [3] made it possible to develop a DPSU program for simulating processes of solid-phase diffusion of silicon in gallium arsenide. For this purpose, we worked out a subprogram DPSJ to obtain a numerical solution to the diffusion equation for silicon [3] over the time interval $[t, \hat{t}]$. Moreover, we worked out a subprogram VLDF to calculate the distributions of intrinsic point defects (neutral vacancies of gallium and neutral vacancies of arsenic in our case). We also developed a number of auxiliary subprograms to calculate the quantity n_i, the reduced concentration of charge carriers χ, the coefficients in the diffusion equation, the initial distributions of silicon atoms in the sublattices of arsenic and gallium, etc.

We note that the approximation of the boundary conditions with the use of fictitious regions [3] permits one to easily realize agreement between the initial and boundary conditions. This is done with a special auxiliary subprogram by calculating the starting values of the concentrations of the impurity at the fictitious points C_0 and C_{m_x+1} from the boundary conditions and the initial distribution of the impurity.

The head module of the DPSU program specifies the sequence of the operation of the subprograms described. During the calculations we input and output the initial data, calculate the distributions of intrinsic point defects (IPD), solve numerically the diffusion equation for silicon atoms for the entire range of heat treatment, and output the results obtained.

Using FORTRAN, we developed two versions of the DPSU program for use in the SVM ES-1061 system and in personal computers of the IBM PC-386 type. The simulation time for a typical process of solid-phase diffusion of silicon on an ES-1061 amounts to about 18 min when using a grid having 241 discretization points for the spatial variable and 300 grid steps.

Without going outside of the required accuracy for the computations (the relative error in the measurement of the concentrational profile of the distribution of the impurity can be taken equal to 5%), the time for the computations can be reduced to 4−5 min by reducing the number of nodes of the spatial-time discretization.

4.2. Results of Numerical Calculations. Using the developed model of solid-phase diffusion of silicon [1, 2], we perform numerical calculations of the process of high-concentration doping of gallium arsenide during thermal diffusion of silicon from a source with a constant concentration of impurity near the semiconductor surface. To check the adequacy of the model, we use experimental data of [4], where the authors investigated the diffusion of silicon into GaAs substrates doped by zinc to a concentration of $10^5 \, \mu m^{-3}$. After purification, a 0.04-μm-thick layer of Si was deposited onto the substrate surface, which was covered with a layer of SiO_2 of thickness 0.1 μm, which served as a protective mask. Heat treatment was carried out in an ampul in an arsenic atmosphere at a
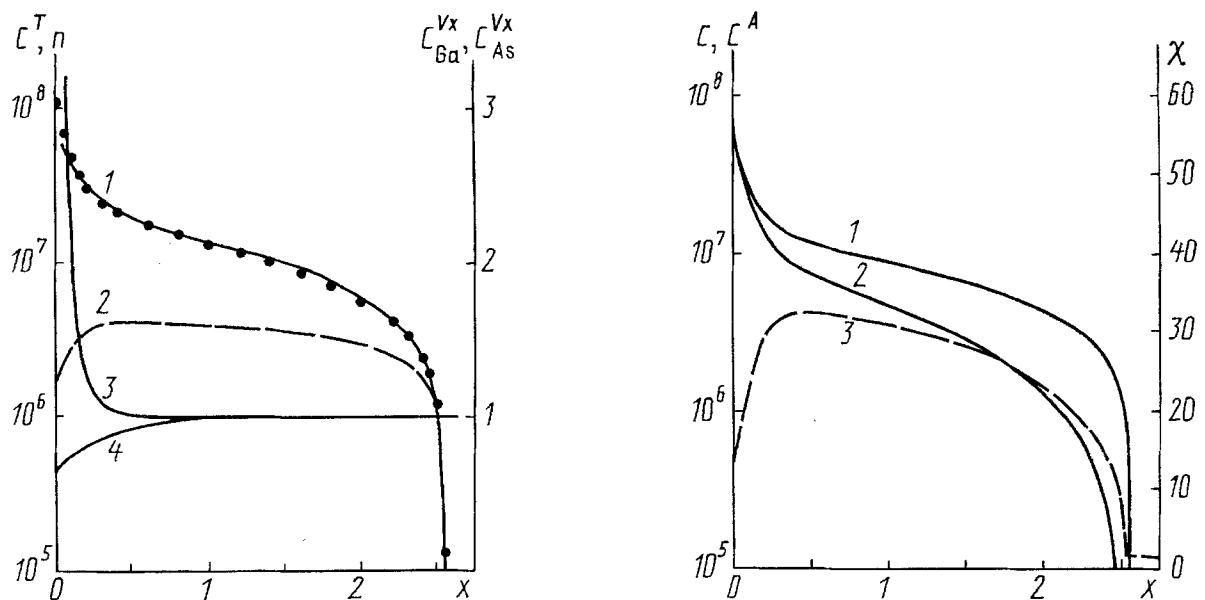
Fig. 1. Distribution of silicon atoms and intrinsic point defects during diffusion from a constant source: 1) measured distribution of the total concentration of silicon atoms (points, predicted distribution of the total concentration of silicon); 2) predicted distribution of the concentration of electrons; 3, 4) calculated distributions of reduced concentrations of neutral vacancies of arsenic and gallium. C^T, μm^{-3}; n, μm^{-3}; C_{As}^{Vx}, C_{Ga}^{Vx}, rel. units.

Fig. 2. Calculated partial distributions of silicon atoms in the sublattices of gallium and arsenic: 1, 2) calculated distributions of silicon atoms in the sublattices of gallium and arsenic; 3) distribution of the reduced concentration of charge carriers χ. C, μm^{-3}; C^A, μm^{-3}; χ, rel. units.

temperature of 850°C for 1428 minutes. The total concentration of silicon atoms was measured by the method of secondary ionic mass-spectroscopy (SIMS). The measured concentration profile of the distribution of silicon is presented in Fig. 1. The figure also contains results of a numerical calculation of the process of solid-phase diffusion of silicon obtained by means of the program developed. In addition to the distribution of the total concentration of the impurity, Fig. 1 also shows the predicted distributions for the concentrations of charge carriers and gallium and arsenic vacancies in a neutral charge state.

The predicted partial distributions of silicon atoms in the gallium and arsenic sublattices are shown in Fig. 2. The distribution of the reduced concentration of charge carriers χ is also presented here.

From Fig. 1 it is seen that the experimental profile of the distribution of silicon has a very complex structure that includes: a portion of a pronounced "ascending" diffusion near the semiconductor surface, an extended portion of a slow fall in the impurity concentration with an "inflection" point at which the second derivative of the total concentration of silicon is equal to zero, and finally a portion of a sharp fall in the impurity concentration deep in the semiconductor. We can see good qualitative and quantitative agreement between results of calculations and experimental data over the entire depth of doping. This is indicative of the adequacy of the proposed model of diffusion and the validity of the assumptions made.

In accordance with experimental data, it was assumed in calculating the distributions of IPD that generation of arsenic vacancies and absorption of gallium vacancies occur near the semiconductor surface [1, 2, 5, 6]. As follows from Eq. (3) or (9) of [2], the formation of the near-surface maximum of the impurity concentration results from a decrease in the concentration of gallium vacancies, as is confirmed by the numerical calculations carried out. Simultaneously, generation of arsenic vacancies on the interface leads, as follows from Eqs. (13) and (15) of [1], to a decrease in the concentration of charge carriers near the semiconductor surface. This phenomenon is confirmed by both experimental data [7, 8] and results of the simulation (see Figs. 1 and 2).

In performing the calculations represented in Figs. 1 and 2, we used the following values of the parameters that characterize the process of transfer of silicon atoms: $n_i = 1.241 \cdot 10^5 \ \mu\text{m}^{-3}$; $\beta_1 = 0$; $\beta_2 = 0$; $\beta_3 = 0.0445$; $\beta_4 = 0$; $D_i = 2.4 \cdot 10^{-8} \ \mu\text{m}^2/\text{sec}$; $C_S^T = 1.141 \cdot 10^8 \ \mu\text{m}^{-3}$ and the state of the defect subsystem of the crystal: $L_{\text{Ga}}^V = 0.3$ μm; $L_{\text{As}}^V = 0.07 \ \mu\text{m}$; $\widetilde{C}_{\text{Ga}}^{Vx}(0) = 0.65$; $\widetilde{C}_{\text{As}}^{Vx}(0) = 6.0$; here the values of the parameters β_3, L_{Ga}^V, L_{As}^V, $\widetilde{C}_{\text{Ga}}^{Vx}(0)$, and $\widetilde{C}_{\text{As}}^{Vx}(0)$ were determined from the condition of the best agreement of predicted results with experimental data.

The attaining agreement with experimental data for a rather complex diffusion process, when the impurity is located at the nodes of both sublattices of the crystal and various effects in the near-surface region are substantial, testifies to the success of the simulation of this process and to a high efficiency of the mathematical program developed.

GENERAL CONCLUSIONS

1. Based on an analysis of experimental data, we showed that transfer of the main quantity of silicon atoms in gallium arsenide is carried out by means of gallium vacancies.

2. We developed a model of transport of silicon atoms between the sublattices of gallium arsenide and identified the parameters of the process for a treatment temperature of 850°C.

3. We developed a model of solid-phase diffusion of silicone with account for the amphoteric behavior of the impurity and nonuniform distribution of arsenic and gallium vacancies. The diffusion equation for silicon was obtained in a form suitable for numerical solution.

4. To solve the diffusion equation for the impurity atoms, we employed a new method of finite-difference approximation permitting one to use "rough" grids for solving equations with highly nonlinear coefficients and large concentration gradients of the impurity.

5. Calculations of the diffusion of silicon demonstrated the adequacy of the model suggested and high efficiency of the mathematical program developed, which makes it possible to calculate the distributions of the impurity in both sublattices of the crystal as well as the gallium and arsenic vacancies.

NOTATION

n_i, concentration of intrinsic charge carriers; D_i, intrinsic coefficient of silicone diffusion in gallium arsenide; V_{Ga}^-, gallium vacancy in the charged state r_{Ga}^-; V_{As}^+, arsenic vacancy in the charged state r_{As}^+; $\times$, sign of the neutral charged state; $\widetilde{C}_{\text{Ga}}^{Vx}$ and $\widetilde{C}_{\text{As}}^{Vx}$, concentrations of gallium and arsenic vacancies reduced to thermally equilibrium values in the neutral charged state; C and C^A, concentrations of atoms at the nodes of the gallium and arsenic sublattices, respectively; C^T, total concentration of silicon atoms; N, concentration of ionized atoms of a different impurity with the opposite type of conductivity; T, temperature; t, time of heat treatment; $D(\chi, T)$, effective coefficient of silicon diffusion in gallium arsenide; χ, reduced concentration of electrons; C_S^T, total concentration of impurity atoms near the semiconductor surface; L_{Ga}^V and L_{As}^V, diffusional mean free paths of gallium and arsenic vacancies, respectively.

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