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MODELING OF SILICON DIFFUSION IN GALLIUM ARSENIDE.
2. DIFFUSION EQUATION

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The equation of diffusion of silicon atoms in gallium arsenide is obtained in a form convenient for numerical solution.

Having identified in [1] the microscopic mechanism of the transfer of silicon atoms and formulated a model of the transitions of impurity atoms between the sublattices of gallium arsenide, we can complete the development of the model for solid-phase diffusion of silicon. For this purpose we will obtain the diffusion equation for impurity atoms.

2.1. The Equation of Diffusion of Silicon Atoms in Gallium Arsenide. In order to derive the equation of diffusion of impurity atoms, the procedure proposed in [2] will be used. We write the equation of diffusion and quasichemical reactions of particles of species α

$$C_t^\alpha = \nabla \left[D^\alpha \left(\omega^\alpha \nabla C^\alpha \frac{\overset{\alpha}{z} e}{k_\mathrm{B} T} E C^\alpha \right) \right] + \sum_{i=1}^{m} \nu^{\alpha i} v_i - S^\alpha + G^{T\alpha} + G^{R\alpha} , \quad \alpha = 1 , 2 , \ldots , l , \tag{1}$$

$$\omega^\alpha = (C^\alpha / (k_\mathrm{B} T)) \, \partial \mu^\alpha / \partial C^\alpha \tag{2}$$

for silicon atoms in the gallium and arsenic sublattices and for complexes of silicon atoms in the gallium sublattice with vacancies of gallium in different charge states (CS). Then we transform the set of equations obtained similarly to [2]. However, unlike [2], on the right-hand side of the equation as many quantities as possible will be introduced under the sign of the second derivative. The derived diffusion equation of silicon atoms in gallium arsenide has the following form:

$$C_t^T = \Delta \left[D \tilde{C}_\mathrm{Ga}^{V\times} C \right] + \nabla \left[\omega^\chi (D - \chi R) (C/\chi) \tilde{C}_\mathrm{Ga}^{V\times} \nabla \chi \right] , \tag{3}$$

$$C^T = C + C^A , \tag{4}$$

$$D (T , \chi) = C_{\mathrm{Ga_i}}^{V\times} \sum_r D_\mathrm{Ga}^{Er-} H_\mathrm{Ga}^{Er-} h_\mathrm{Ga}^{Vr-} \chi^{-zz_\mathrm{Ga}^{Vr-}} , \tag{5}$$

$$R (T , \chi) = C_{\mathrm{Ga_i}}^{V\times} \sum_r \left(- zz_\mathrm{Ga}^{Vr-}\right) D_\mathrm{Ga}^{Er-} H_\mathrm{Ga}^{Er-} h_\mathrm{Ga}^{Vr-} \chi^{-(zz_\mathrm{Ga}^{Vr-} + 1)} , \tag{6}$$

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$$\chi = \frac{C - C^A - N + \sqrt{(C - C^A - N)^2 + 4n_{ie}^2}}{2n_i}, \tag{7}$$

$$C^A = A\chi^2 C. \tag{8}$$

Let us consider the differences between Eq. (3) for the diffusion of silicon atoms and the generalized equation in [2]. The diffusion equation from [2] will be expressed as

$$C_t^T = \nabla\, [\, D\, \nabla\, (\tilde{C}_{\mathrm{Ga}}^{V\times}\, C\,)\,] + \nabla\, [\, D\tilde{C}_{\mathrm{Ga}}^{V\times}\, (C/\chi)\, \nabla\chi\,]. \tag{9}$$

It is seen from (3) and (9) that Eq. (9) is more convenient for qualitative investigation of the physics of the diffusion process, because under the sign of the gradient we have the product of the concentration of the neutral IPD (intrinsic point defects) by the concentration of the impurity atoms in the substitution position. On the other hand, diffusion equation (3) is more convenient for performing numerical calculations. Indeed, the second term on the right-hand side of Eq. (3), as a rule, is substantially smaller in absolute value than a similar term in Eq. (9). Moreover, we can write:

$$\nabla\, [\, \omega^\chi\, (D - \chi R)\, \tilde{C}_{\mathrm{Ga}}^{V\times}\, \nabla\chi\,] = \nabla\, [\, \omega^\chi\, (D - \chi\, R)\, \tilde{C}_{\mathrm{Ga}}^{V\times}\, h^B\, \nabla\, (C - C^A)\,] -$$

$$- \nabla\, [(\nabla N)\, \omega^\chi\, (D - \chi R)\, \tilde{C}_{\mathrm{Ga}}^{V\times}\, h^B\,], \tag{10}$$

$$\nabla\, [\, D\, (C/\chi)\, \tilde{C}_{\mathrm{Ga}}^{V\times}\, \nabla\chi\,] = \nabla\, [\, D\tilde{C}_{\mathrm{Ga}}^{V\times}\, h^B\, \nabla\, (C - C^A)\,] - \nabla\, [\, (\nabla N)\, D\tilde{C}_{\mathrm{Ga}}^{V\times}\, h^B\,], \tag{11}$$

$$h^B = (C - C^A)/\sqrt{(C - C^A - N)^2 + 4n_{ie}^2}\,. \tag{12}$$

Then from expressions (10) and (11) it is evident that the second terms on the right-hand sides of Eqs. (3) and (9) can be expressed as two components with the second component proportional to the concentration gradient C of the impurity atoms. With a sharply nonuniform distribution of the second impurity, i.e., at large ∇N, these components can also be sufficiently large. In this case in Eq. (9) the term proportional to ∇C can exceed the term $\nabla[D\nabla(\tilde{C}_{\mathrm{Ga}}^{V\times}C)]$ in absolute value. This complicates the construction of an adequate finite-difference scheme of second order of accuracy in spatial coordinates [3]. This disadvantage is not so pronounced when using Eq. (3), since the value of the second term on the right-hand side of this equation is essentially smaller. Moreover, the presence of the term $\Delta[D\tilde{C}_{\mathrm{Ga}}^{V\times}C]$ on the right-hand side of (3) makes it possible to apply the new approach to numerical solution of unsteady-state partial equations with nonlinear coefficients [4], whereas in the case of diffusion equation (9) it is difficult.

2.2. Analysis of the Coefficients in the Equation of Diffusion of Silicon Atoms in Gallium Arsenide. Now let us express the coefficients D and R of Eq. (3) in a form convenient for modeling technological processes. We take into consideration that, according to the microscopic mechanism considered, the impurity atoms are transferred by neutral and negatively charged vacancies of gallium. We assume that no more than fourfold charged defects participate in the diffusion of the impurity and take into account that $z = +1$. Then expressions (5) and (6) may be expressed as

$$D\,(T\,,\,\chi) = D_i\,(1 + \beta_1\chi + \beta_2\chi^2 + \beta_3\chi^3 + \beta_4\chi^4)/\beta_0\,, \tag{13}$$

$$R\,(T\,,\,\chi) = D_i\,(\beta_1 + 2\beta_2\chi + 3\beta_3\chi^2 + 4\beta_4\chi^3)/\beta_0\,, \tag{14}$$

$$D_i = D_i^{\times} + D_i^{-} + D_i^{2-} + D_i^{3-} + D_i^{4-}, \tag{15}$$

$$\beta_0 = 1 + \beta_1 + \beta_2 + \beta_3 + \beta_4, \tag{16}$$

$$\beta_r = D_i^{r-}/D_i^{\times} = (D_{\mathrm{Ga}}^{Er-}\, H_{\mathrm{Ga}}^{Er-}\, h_{\mathrm{Ga}}^{Vr-})/(D_{\mathrm{Ga}}^{E\times}\, H_{\mathrm{Ga}}^{E\times}\, h_{\mathrm{Ga}}^{V\times}). \tag{17}$$

It will be assumed that D_{Ga}^{Er-}, H_{Ga}^{Er-}, and h_{Ga}^{Vr-} are functions of the process temperature alone. Then β_r are also functions of the process temperature and can be determined from the experimentally measured dependence of the diffusion coefficient on the concentration. In the case of the absence of this dependence, β_r can be considered as fitting parameters in modeling the diffusion process.

One can see from expressions (13) to (17) that at the prescribed temperature of the process the form of the power dependence function of the diffusion coefficient $D = D(\chi)$ and of the product $\chi R(\chi)$ is directly proportional to the charge state of the IPD. It will be taken into consideration that triply charged vacancies of gallium V_{Ga}^{3-} participate in the transfer of silicon atoms [5]. Hence, it follows that the dependence of the effective diffusion coefficient $D(\chi)$ on the impurity concentration is determined by a polynomial in χ at least to the third power (at $C >> n_i\, \chi \approx C/n_i$).

The result obtained implies that the effective transfer coefficients $D(T, \chi)$ and $R(T, \chi)$ in Eq. (3) are strongly nonlinear functions of the concentration C of silicon atoms in the gallium sublattice. Moreover, as follows from Eq. (13) (see [1]), the dependence of the concentration of silicon atoms in the arsenic sublattice is also a strongly nonlinear function in a particular range of $C^A = C^A(C)$.

The strongly nonlinear dependences of the coefficients $D(T, \chi)$ and $R(T, \chi)$ and the function $C^A = C^A(C)$ hinder numerical solution of Eq. (3) [3]. Therefore, to solve diffusion equation (3), we used the new approach to the construction of difference schemes [4], intended for coarse finite difference solution of unsteady-state problems with specific features (large gradients, a strong nonlinear dependence of the equation coefficients, etc.). The present calculations of diffusion of arsenic in silicon have shown the high efficiency of this method in the numerical solution of diffusion equations [6].

NOTATION

n_i and n_{ie}, concentration of intrinsic charge carriers and its effective value at high doping levels; D_i, intrinsic coefficient of diffusion of silicon in gallium arsenide; V_{Ga}^{r-}, vacancy of gallium in the charge state r_{Ga}^{-}; V_{As}^{r+}, vacancy of arsenic in the charge state r_{As}^{+}; C_{Ga}^{Vr-} and C_{As}^{Vr+}, concentrations of these particles; ×, sign of neutral charge state; $C_{\mathrm{Ga}_i}^{V\times}$ and $C_{\mathrm{As}_i}^{V\times}$, thermal-equilibrium values of the vacancy concentrations of gallium and arsenic in the neutral charge state; e^-, electron; C and C^A, concentrations of atoms at gallium sublattice point and arsenic sublattice point, respectively; C^T, total concentration of silicon atoms; N, concentration of ionized atoms of the other impurity of the opposite type of conductivity; C^{α}, D^{α}, μ^{α}, and z^{α}, concentration, diffusion coefficient, chemical potential, and particle charge of species α, respectively; $\nu^{\alpha i}$, quantity of particles of species α formed in the quasichemical reaction of the ith kind; v_i, rate of this reaction; S^{α}, absorption rate of the particles of species α by fixed disturbances of the crystal lattice; $G^{T\alpha}$ and $G^{R\alpha}$, rate of heat generation of these particles and the rate of their generation rate as a result of external irradiation; e, electron charge; k_{B}, Boltzmann constant; T, temperature; t, time of thermal treatment; h_{Ga}^{r-} and h_{As}^{r+}, constants of local thermodynamic equilibrium for reactions of transition of gallium vacancies and arsenic vacancies from the neutral state to the charged states r^- and r^+, respectively; $D(\chi, T)$, effective coefficient of diffusion of silicon in gallium arsenide; D_{Ga}^{Er-}, coefficient of diffusion of the complex formed by a silicon atom at the gallium sublattice point $\mathrm{Si}_{\mathrm{Ga}}^{+}$ and vacancy V_{Ga}^{r-}; H_{Ga}^{Er}, constant of local equilibrium for the reaction of formation of these complexes; z and z_{Ga}^{Vr-}, charges of the silicon atom in the gallium sublattice $\mathrm{Si}_{\mathrm{Ga}}^{+}$ and gallium vacancy V_{Ga}^{r-}, expressed in electron charge units; χ, reduced concentration of electrons; ω^{χ}, function, describing the deviation of the state of electron gas from the ideal one at high doping levels; $D_i^{\times}$ and D_i^{r-}, partial coefficients of diffusion of silicon in low-doped gallium arsenide by means of complexes ($Si_{Ga}^{+}V_{Ga}^{\times}$) and $Si_{Ga}^{+}V_{Ga}^{r-}$); *E*, internal electric field vector.

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