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# MODELING OF DIFFUSION OF MAGNESIUM IN GALLIUM ARSENIDE. 1. THERMAL DIFFUSION OF Mg IN $Al_xGa_{1-x}As$

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*A model is developed and an equation is derived for magnesium diffusion in gallium arsenide. Numerical modeling of $Al_xGa_{1-x}As$ doping has shown that the suggested model makes it possible to adequately describe all distinctive features of the profile of magnesium atom distribution in thermal diffusion.*

At present gallium arsenide-based and $Al_xGa_{1-x}As$-based integrated circuits (IC) and devices find ever-increasing application in computer equipment and SHF technology. This is due to the higher mobility of charge carriers than in silicon and, therefore, the higher speed of response of devices and ICs. At the same time these materials have been less thoroughly studied than silicon, which is a serious handicap in developing technological processes, in particular, processes of local doping of semiconductor substrates.

The present work is aimed at investigating and developing a model of diffusion processes for magnesium in GaAs and $Al_xGa_{1-x}As$.

Magnesium is an important acceptor impurity used currently for the manufacture of devices based on gallium arsenide. But Mg diffusion is a more complicated process than the diffusion of other acceptor impurities. In Fig. 1a profile of Mg distribution in $Al_{0.2}Ga_{0.8}As$ is shown for diffusion from a constant source [3]. Doping was accomplished at 785°C from liquid Ga saturated with As and containing 0.11 wt.% Mg. The time of treatment was 20 min. As is seen, the profile of Mg distribution has a complicated structure including: a) a near-surface region of abrupt decrease of the concentration of impurity atoms; b) a point of "inflection" where the second derivative of the impurity concentration is equal to zero; c) an extended "tail" in the low-concentration region of the impurity.

To construct a diffusion model, we shall identify at first the microscopic transfer mechanism for impurity atoms. For this, we analyze the basic regularities of Mg diffusion in complex semiconductors. Since substitutional magnesium atoms are negatively charged, neutral and positively charged defects may take part in the transfer of impurity atoms. The charge state of the defect participating in the transfer of impurity atoms may be determined from the form of the concentration dependence of the diffusion coefficient. Since the diffusion process is accomplished from a constant source [3], we may use the Boltzmann–Matano method to determine this dependence. An analysis of experimental data [3] by this method has shown that the diffusion coefficient is proportional to the third power of the hole concentration. This means that triply charged defects participate in the transfer of the main amount of the impurity. In gallium arsenide the positively charged intrinsic point defects are the interstitial gallium atoms $I_{Ga}^{m+}$, with $m$ being, in all probability, equal to 3 [4], and arsenic vacancies $V_{As}^{2+}$ [5]. A positive charge on the interstitial arsenic atoms must not be ruled out.

We now show that the magnesium atoms are most likely transferred by the interstitial gallium atoms $I_{Ga}^{3+}$. Actually, the process of magnesium diffusion is retarded with an increase in the arsenic vapor pressure [6], i.e., upon supersaturation of a semiconductor with interstitial arsenic atoms $I_{As}$. This means that they do not participate in transfer of the main amount of impurity atoms. On the other hand, this retardation of diffusion is consistent with the assumption of the participation of interstitial atoms in the magnesium transfer processes since supersaturation of the semiconductor with arsenic atoms $I_{As}$ entails a decrease in the concentration of interstitial gallium atoms [4, 7].

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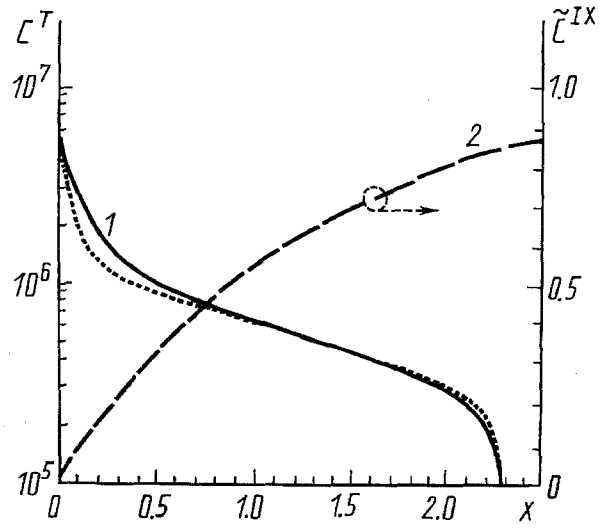


Fig. 1. Distribution of magnesium atoms and intrinsic point defects in diffusion from a constant source: 1) measured distribution of the total concentration of magnesium atoms [3] (the dotted line is the calculated distribution of the total magnesium concentration); 2) calculated distribution of the reduced concentration of interstitial atoms of elements of group III in the neutral charge state. $C^T$, $\mu m^{-3}$; $\tilde{C}^{Ix}$, rel. units.

Next, we consider the possibility of transfer of Mg atoms by positively charged arsenic vacancies. As is seen from Fig. 1, the profile of the magnesium distribution is qualitatively similar to the phosphorus distribution in silicon in high-concentration diffusion. Therefore the characteristic features of the magnesium and phosphorus distribution profiles may be explained by the nonuniform distribution of intrinsic point defects (IPD) responsible for the transfer of impurity atoms. This nonuniform distribution is due to defect absorption by the surface of gallium arsenide. Apparently, such an assumption is quite reasonable for interstitial gallium atoms and hardly tenable for arsenic vacancies since a phase interface, according to [8], is a source of arsenic vacancies rather than a sink of these defects. This means that the most probable type of defects providing transfer of the main amount of Mg atoms in gallium arsenide is interstitial gallium atoms.

We now consider magnesium diffusion in $Al_xGa_{1-x}As$. It is assumed that along with interstitial atoms $I_{Ga}$ the semiconductor lattice possesses interstitial aluminum atoms $I_{Al}$ [7]. But both aluminum and gallium are group III elements. This means that interstitial aluminum atoms may also participate in the transfer of magnesium atoms. Taking into consideration the distinctive features of $Al_xGa_{1-x}As$, we shall assume that interstitial atoms of elements of group III, i.e., gallium and aluminum, take part in the transfer of magnesium atoms.

Having identified the microscopic mechanism, we may construct a quantitative model of magnesium diffusion. In accordance with the results of the analysis, we assume that transfer of magnesium atoms is a result of formation, migration, and decay of complexes of a substitutional magnesium atom and an interstitial atom of an element of group III ($Mg_{Ga}^{-} - I_{III}^{m+}$). Then the equation for magnesium diffusion may be represented as [9]:

$$C_t^T = \nabla\,[D\nabla\,(\tilde{C}^{Ix} C)] + \nabla\,[D\tilde{C}^{Ix} C\nabla\chi/\chi]\,, \tag{1}$$

$$D(\chi) = D_i(1 + \beta_1\chi + \beta_2\chi^2 + \beta_3\chi^3)/\beta_i\,,$$

$$\chi = \frac{C - N + \sqrt{(C-N)^2 + 4n_i^2}}{2n_i}\,,$$

$$\tilde{C}^{Ix} = C^{Ix}/C_i^{Ix}\,, \quad D_i = D_i^{\times} + D_i^{+} + D_i^{2+} + D_i^{3+}\,, \quad \beta_q = D_i^q/D_i^{\times}\,.$$

As is seen from Eq. (1), unlike the equation of Fick's second law, the flux of impurity atoms is determined not only by the gradient of the impurity concentration but also by the gradient of the product of the atomic impurity concentration and the concentration of interstitial atoms of elements of group III in the neutral charge state. The numerical solution of the diffusion boundary-value problem given below shows that this distinctive feature of the equation makes it possible to describe a particular form of magnesium distribution by introducing just the assumption of the absorption of interstitial atoms of elements of group III by the semiconductor surface.

To solve numerically the diffusion equation for magnesium atoms, we use the finite-difference method. For this, we reduce Eq. (1) to the form

$$C_t^T = \nabla\,[D\tilde{C}^{I\times} C] + \nabla\,[(D - R\chi)\,\tilde{C}^{I\times} C\nabla\chi/\chi]\,, \tag{2}$$

$$R(\chi) = D_i(\beta_1 + 2\beta_2\chi + 3\beta_3\chi^2)/\beta_i\,.$$

As seen from Eq. (2), for the finite-difference approximation of the first (main) term in the right-hand side of the equation there is no need to calculate quantities between grid nodes. This facilitates numerical solution of the diffusion equation substantially. Considering that the concentration dependence of the diffusion coefficient is determined, as judged from an analysis of the profile of the magnesium distribution by the Boltzmann–Matano method, by a third-degree polynomial, we use the method of constructing finite-difference schemes [10] to approximate Eq. (2). This method permits nonstationary boundary-value problems that are distinguished by some special features (large gradients of a solution, a substantially nonlinear dependence of the coefficients in the equation, and so on) to be solved numerically using "rough" grids.

To solve Eq. (2), it is necessary to know the distribution of the reduced concentration of interstitial atoms of elements of group III in the neutral charge state $\tilde{C}^{I\times}$. This distribution may be obtained from a solution of the diffusion equation for intrinsic interstitial atoms [11]. To obtain an analytical solution, we represent this equation in the following form:

$$\Delta\tilde{C}^{I\times} - \tilde{C}^{I\times}/(L^I)^2 + \tilde{C}_g^I/(L^I)^2 = 0\,, \tag{3}$$

$$L^I = \left(D^{I^*}\tau^{I^*}\right)^{1/2}, \quad \tilde{C}_g^I = (g^{I^*}/g_i^I)\,(\tau^{I^*}/\tau_i^I)\,.$$

The doping process depicted in Fig. 1 was modeled by solving numerically the diffusion equation (2) for the impurity and solving analytically the diffusion equation (3) for the defects. In the calculations, use was made of the following values of the parameters characterizing the transfer process for impurity atoms: $n_i = 3.406\cdot10^4$ $\mu m^{-3}$; $D_i = 5.370\cdot10^{-6}$ $\mu m^2/sec$; $\beta_3 = 0.136$; $\beta_1 = \beta_2 = 0$; the state of the defect subsystem of the crystal $L^I = 1.25$ $\mu m$; $\tilde{C}_s^{I\times} = 0.014$. The intrinsic concentration of carriers was determined in accordance with the expression suggested in [12], and the remaining parameters were determined from the condition of the best agreement of the calculated profile of the impurity distribution with the experimental data. Calculation results for the profiles of the distribution of the impurity and the interstitial atoms of elements of group III are presented in Fig. 1.

It should be borne in mind that the profile of the impurity distribution has a complicated form that fails to be described within the framework of Fick's second law. Therefore the fact that the calculation results agree qualitatively and quantitatively with the experimental data points to the adequacy of the developed model of transfer processes for impurity atoms and point defects. It is pertinent to note that in the investigated impurity concentration range the diffusion coefficient of magnesium $D(\chi)$ changes by more than a factor of $3\cdot10^5$. Nevertheless the numerical solution is obtained with a small number of nodes of a uniform grid (101). This is indicative of the high efficiency of the program of numerical solution of the diffusion equation.

Using the suggested model and developed software it is possible to model both thermal diffusion and redistribution processes for ion-implanted magnesium in postimplantation heat treatments. Results of these studies will be published in the second part of our work.

## NOTATION

$I_{Ga}^{m+}$, interstitial gallium atom in the charge state $m^+$; $n_i$, natural concentration of charge carriers; $Mg_{Ga}$, Mg atom in the gallium sublattice; $C^T$, total concentration of magnesium atoms; $C$, concentration of substitutional magnesium atoms; $N$, concentration of the impurity of the opposite type of conduction; $\tilde{C}^{I\times}$, reduced concentration of interstitial atoms of elements of group III in the neutral charge state; $C^{I\times}$, $C_L^{I\times}$, concentration of these particles and its thermal equilibrium value; $D(\chi)$, effective diffusion coefficient of magnesium in gallium arsenide; $\chi$, reduced electron concentration; $D_i$, intrinsic value of the diffusion coefficient of magnesium in gallium arsenide; $D_i^{\times}$, $D_i^{q+}$, partial coefficients of magnesium diffusion in gallium arsenide by means of the complexes $(Mg_{Ga}^{-} - I_{III}^{\times})$ and $(Mg_{Ga}^{-} - I_{III}^{q+})$; $L^I$, mean diffusion length of interstitial atoms of elements of group III; $\tilde{C}_s^{I\times}$, surface value of the reduced concentration of interstitial atoms of elements of group III in the neutral charge state; $D^{I^*}$, $\tau^{I^*}$, $g^{I^*}$, effective values of the diffusion coefficient, lifetime, and rate of generation of interstitial atoms of elements of group III, respectively; $t$, time of heat treatment.

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