Journal of Engineering Physics and Thermophysics, Vol. 68, No. 1, 1995

MODELING OF MAGNESIUM DIFFUSION IN GALLIUM ARSENIDE.
2. REDISTRIBUTION OF ION-IMPLANTED IMPURITY

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UDC 53.01.072:681.3

The redistribution of ion-implanted magnesium under high-rate annealing conditions is calculated. Consideration of the nonuniformity of the interstitial gallium atom distribution makes it possible to explain "ascending" diffusion in the region of strong distortions of a crystalline lattice.

Calculations of the magnesium distribution profile made in the first part of our work [1] have shown that the suggested model adequately describes thermal diffusion of magnesium upon doping from a constant source. Therefore the developed model may be used in modeling different diffusion processes of magnesium.

At present, ion implantation finds wide application for creating local doped sites in the manufacture of gallium arsenide devices. In this case the final impurity distribution is determined by both the ion implantation parameters and the diffusion redistribution of impurity atoms during postimplantation annealing. We shall consider the redistribution of magnesium atoms in the case of high-rate annealing of semiconductor substrates [2]. In [2] undoped semiinsulating GaAs was implanted with magnesium 150 keV ions at a rate of 10^6 ion/μm^2. Annealing was performed for 2 min at 900°C. To decrease impurity evaporation, a Si_3N_4 layer was deposited. Magnesium distribution profiles measured by the SIMS method are given in Fig. 1.

As is seen, after annealing, the magnesium distribution profile has a complicated structure that includes an "ascending" diffusion region near the maximum of the impurity concentration. The presence of such a region is a characteristic feature of the redistribution of ion-implanted magnesium that is not observed in redistribution of other impurities [2].

In order to explain the phenomenon of "ascending" magnesium diffusion, in [2] the defect generation upon implantation of magnesium and beryllium ions was calculated. It was found that magnesium implantation results in more substantial generation of interstitial gallium atoms than implantation of other impurities. It has been supposed that "ascending" Mg diffusion is caused by nonuniform distribution of a large amount of nonequilibrium interstitial gallium atoms. The modeling of magnesium atom redistribution performed in [2] has shown that use of the assumptions made allows one to achieve good agreement between the calculated impurity distribution profile and the experimental data, including the "ascending" diffusion region. For modeling the impurity redistribution with nonuniform distribution of interstitial gallium atoms use has been made of the SUPREM-IV program based on the model of impurity diffusion by formation of impurity atom-intrinsic point defect pairs [3]. The microscopic mechanism of diffusion by processes of formation, migration, and decay of impurity atom-intrinsic point defect complexes was suggested for the first time in [4], where the basic diffusion equations are derived.

Despite the consistency with experimental data, the mechanism of formation of the region of "ascending" impurity diffusion proposed in [2] has an essential drawback. The issue is that within the framework of the suggested model the "ascending" diffusion process occurs, as follows from calculations presented in that work, only in the absence of diffusion of interstitial gallium atoms. Thus, for the parameters of migration of interstitial gallium atoms used in [2] we have calculated that the diffusion mean free path of these defects in the intrinsic semiconductor does not exceed 0.004 μm. At the same time it is known that the intrinsic interstitial atoms have

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Belarusian State University of Information Science and Radioelectronics, Minsk, Belarus. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 68, No. 1, pp. 39-43, January-February 1995. Original article submitted September 22, 1993.

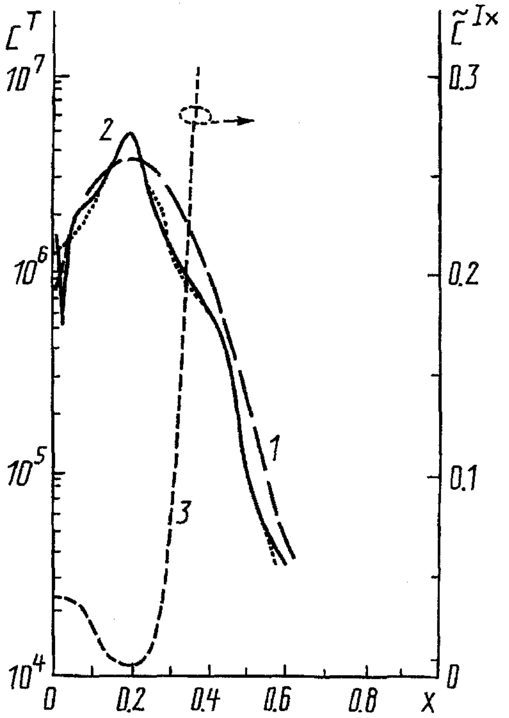

Fig. 1. Distribution of magnesium atoms and intrinsic point defects upon diffusion of an ion-implanted impurity: 1) measured distribution of the total magnesium atom concentration after implantation [2]; 2) measured distribution of the total magnesium atom concentration after annealing [2] (points, the total magnesium concentration distribution calculated in the present work); 3) calculated distribution of the reduced concentration of interstitial gallium atoms in a neutral charge state. C^T, $\mu\mathrm{m}^{-3}$; $\tilde{C}^{I\times}$, rel. units.

substantially higher mobility than the interstitial impurity atoms [5, 6]. It should be expected that the diffusion mean free path of these defects will be substantially larger than the above value.

To eliminate this contradiction, we assume that a nonuniform distribution of interstitial gallium atoms is formed in the following way. In the initial stage of high-rate annealing, implanted primary radiation defects are redistributed beyond the layer of the implanted impurity. Due to decay of these defects a large amount of interstitial gallium atoms are generated, which supersaturates the semiconductor volume with intrinsic interstitial atoms and accelerates the diffusion process in the impurity region. Such a mechanism of redistribution and generation of defects is confirmed by results of measurement of the spatial defect distribution in ion-implanted layers [7, 8]. Proceeding from this mechanism of redistribution of primary radiation-induced defects, we assume, unlike [2], that the generation rate of nonequilibrium interstitial gallium atoms is approximately the same within the doped layer. On the other hand, in the region of the most substantial distortions of the crystal lattice there is intense formation of secondary radiation-induced defects. These defects may include packing defects, dislocation loops, and other defects of interstitial type [9–11]. This process is accompanied by intense local absorption of intrinsic interstitial atoms. Moreover, interstitial gallium atoms may be absorbed as a result of their interaction with the semiconductor surface. The last two processes are responsible for the nonuniform distribution of interstitial gallium atoms in the doped layer.

To calculate the nonuniform distribution of interstitial gallium atoms we subdivide the semiconductor volume into three regions whose boundariers have the coordinates $[0, x_L]$, $[x_L, x_R]$, $[x_R, x_F]$. Here x_L and x_R are the boundaries of the region where interstitial atoms are absorbed intensely; x_F is the boundary of the region of modeling the impurity redistribution process. In conformity with the assumptions made we consider the three indicated regions to have different absorption rates of interstitial gallium atoms and, consequently, to be characterized by different lifetimes (τ_1, τ_2, τ_3) and mean free paths (l_1, l_2, l_3) of interstitial gallium atoms.

In this case the analytical solution of the diffusion equation of interstitial gallium atoms (3), given in the first part of our work [1], is as follows:

$$\tilde{C}_n^{I\times}(x) = \tilde{C}_{gn} + C_{1n}\exp(-x/l_n) + C_{2n}(x/l_n)\,, \tag{1}$$

where

$$C_{11} = \frac{(W_3 - W_2\tilde{C}_{g1})\exp(x_L/l_1) - (W_2 + W_1/l_1)(C_L - \tilde{C}_{g1})}{\Delta_1}\,;$$

$$C_{21} = \frac{-(W_3 - W_2\tilde{C}_{g1})\exp(-x_L/l_1) + (W_2 - W_1/l_1)(C_L - \tilde{C}_{g1})}{\Delta_1}\,;$$

$$C_{12} = \frac{(C_L - \tilde{C}_{g2})\exp(x_R/l_2) - (C_R - \tilde{C}_{g2})\exp(x_L/l_2)}{\Delta_2}\,;$$

$$C_{22} = \frac{-(C_L - \tilde{C}_{g2})\exp(-x_R/l_2) + (C_R - \tilde{C}_{g2})\exp(-x_L/l_2)}{\Delta_2}\,;$$

$$C_{13} = (C_R - \tilde{C}_{g3})\exp(x_R/l_3)\,;$$

$$C_{23} = 0\,;$$

$$C_L = \Delta_L/\Delta\,;$$

$$C_R = \Delta_R/\Delta\,;$$

$$\Delta_L = \left\{\frac{1}{l_1\Delta_1}\left[2(W_3 - W_2\tilde{C}_{g1}) + (W_2 - W_1/l_1)\tilde{C}_{g1}\exp(x_L/l_1) + \right.\right.$$

$$\left. + (W_2 + W_1/l_1)\tilde{C}_{g1}\exp(-x_L/l_1)\right] + \frac{\tilde{C}_{g2}}{l_2\Delta_2}\left[\exp((x_R - x_L)/l_2) + \right.$$

$$\left.\left. + \exp(-(x_R - x_L)/l_2) - 2\right]\right\}\left\{1/l_3 + \frac{1}{l_2\Delta_2}\left[\exp((x_R - x_L)/l_2) + \right.\right.$$

$$\left.\left. + \exp(-(x_R - x_L)/l_2)\right]\right\} + \frac{2}{l_2\Delta_2}\left\{\frac{\tilde{C}_{g2}}{l_2\Delta_2}\left[\exp((x_R - x_L)/l_2) + \right.\right.$$

$$\left.\left. + \exp(-(x_R - x_L)/l_2) - 2\right] + \tilde{C}_{g3}/l_3\right\}\,;$$

$$\Delta_R = \left\{\frac{1}{l_1\Delta_1}\left[(W_2 - W_1/l_1)\exp(x_L/l_1) + (W_2 + \right.\right.$$

$$\left. + W_1/l_1)\exp(-x_L/l_1)\right] + \frac{1}{l_2\Delta_2}\left[\exp((x_R - x_L)/l_2) + \right.$$

$$\left.\left. + \exp(-(x_R - x_L)/l_2)\right]\right\}\left\{\frac{\tilde{C}_{g2}}{l_2\Delta_2}\left[\exp((x_R - x_L)/l_2) + \right.\right.$$

$$\left.\left. + \exp(-(x_R - x_L)/l_2) - 2\right] + \tilde{C}_{g3}/l_3\right\} + \frac{2}{l_2\Delta_2}\left\{\frac{1}{l_1\Delta_1}\left[2(W_3 - \right.\right.$$

$$- W_2\tilde{C}_{g1}) + (W_2 - W_1/l_1)\,\tilde{C}_{g1}\exp(x_L/l_1) + (W_2 +$$

$$+ W_1/l_1)\,\tilde{C}_{g1}\exp(-x_L/l_1)\,] + \frac{\tilde{C}_{g2}}{l_2\Delta_2}\,[\exp((x_R - x_L)/l_2) +$$

$$\left. + \exp(-(x_R - x_L)/l_2) - 2\,]\right\};$$

$$\Delta = \left\{\frac{1}{l_1\Delta_1}\,[(W_2 - W_1/l_1)\exp(x_L/l_1) + (W_2 +\right.$$

$$+ W_1/l_1)\exp(-x_L/l_1)\,] + \frac{1}{l_2\Delta_2}\,[\exp((x_R - x_L)/l_2) +$$

$$\left. + \exp(-(x_R - x_L)/l_2)\,]\right\}\left\{\frac{1}{l_2\Delta_2}\,[\exp((x_R - x_L)/l_2) +\right.$$

$$\left. + \exp(-(x_R - x_L)/l_2)\,] + 1/l_3\right\} - \left[\frac{2}{l_2\Delta_2}\right]^2;$$

$$\Delta_1 = (W_2 - W_1/l_1)\exp(x_L/l_1) - (W_2 + W_1/l_1)\exp(-x_L/l_1);$$

$$\Delta_2 = \exp((x_R - x_L)/l_2) - \exp(-(x_R - x_L)/l_2).$$

Here the boundary condition on the semiconductor surface ($x = 0$) is given as a condition of the third kind:

$$W_1\,[\tilde{C}_1(0)\,]_x + W_2\,\tilde{C}_1(0) = W_3\,, \tag{2}$$

where W_1, W_2, W_3 are prescribed constant quantities determined by processes on the semiconductor surface. The boundary condition inside the semiconductor is

$$\tilde{C}_3(x_F) = \tilde{C}_{g3}\,. \tag{3}$$

In modeling the redistribution of ion-implanted magnesium we use this solution (1) to calculate the distribution of interstitial gallium atoms in a neutral charge state.

Our results of modeling the magnesium redistribution for high-rate annealing are shown in Fig. 1.

To describe magnesium diffusion, we used diffusion equation (2) derived in the first part of our work [1]. In the calculations, we used the following values of parameters characterizing the initial distribution of impurity atoms: $R_p = 0.2\ \mu\text{m}$, $\Delta R_p = 0.107\ \mu\text{m}$, Sk = 0.0; for transfer of impurity atoms: $n_i = 1.970\cdot 10^5\ \mu\text{m}^{-3}$, $D_i = 6.507\cdot 10^{-6}\ \mu\text{m}^2/\text{sec}$, $\beta_1 = \beta_2 = 0$, $\beta_3 = 0.135$ and for the state of the defect subsystem of the crystal: $x_L = 0.147\ \mu\text{m}$, $x_R = 0.307\ \mu\text{m}$, $l_1^I = 0.25\ \mu\text{m}$, $l_2^I = 0.1\ \mu\text{m}$, $l_3^I = 0.89\ \mu\text{m}$. The diffusion equation was solved numerically using 61 space discretization nodes with 240 time steps. The results of the same calculations but with use of 121 nodes with 480 time steps differ by 0.2 to 0.5%.

As seen from Fig. 1, the calculation results for the ion-implanted magnesium redistribution agree well with experimental data, including those for the region with "ascending" impurity diffusion. This means that the suggested model describes adequately both the quantitative and qualitative characteristics of redistribution of ion-implanted magnesium upon high-rate annealing. Unlike [2], it is assumed that in the case of annealing, diffusion of intrinsic interstitial gallium atoms takes place and is characterized by reasonable diffusion mean free paths of the defects.

CONCLUSIONS

1. A diffusion model is constructed for magnesium atoms with a nonequilibrium state and nonuniform distribution of intrinsic point defects in GaAs and $Al_xGa_{1-x}As$ crystals.

2. Calculation results have shown that the suggested model describes the processes of both thermal diffusion from a constant source and redistribution of ion-implanted magnesium annealed at high rates. The model is in qualitative and quantitative agreement with experimental data.

3. The developed mathematical apparatus makes it possible to solve numerically the diffusion equation at a high degree of nonlinearity of the equation coefficients when the diffusion coefficient changes by a factor of 10^5 or more [1].

NOTATION

n_i, natural concentration of charge carriers; D_i, eigenvalue of the magnesium diffusion coefficient in gallium arsenide; $\tilde{C}_n^{I\times}(x)$, reduced concentration of intrinsic interstitial gallium atoms in a neutral charge state in the n-th subregion, $n = 1, 2, 3$; l_n^I, diffusion mean free paths of these particles; R_p, Δ_p, Sk, ion impantation parameters: mean projective range of ions, straggling of this range, and parameter of the profile asymmetry of impurity distribution after ion implantation of the latter.

REFERENCES

1. V. A. Labunov, O. I. Velichko, and S. K. Fedoruk, Inzh.-Fiz. Zh., 67, Nos. 5-6, 433-436 (1994).
2. H. G. Robinson, M. D. Deal, G. Amaratunga, et al., J. Appl. Phys., 71, No. 6, 2615-2623 (1992).
3. M. Orlowski, Appl. Phys. Lett., 53, No. 14, 1323-1325 (1988).
4. O. I. Velichko, Radiotekh. Élektron., Republican Interbranch Collected Papers, Issue 14, 91-94, Minsk (1985).
5. V. V. Emtsev and T. V. Mashovets, Impurities and Point Defects in Semiconductors [in Russian], Moscow (1981).
6. J. Boorguen and M. Lanno, Point Defects in Semiconductors. Some Experimental Aspects [Russian translation], Moscow (1985).
7. D. Baither, H. Bartsch, and D. Panknin, Energy Pulse and Particle Beam Modification of Materials: Int. Conf., Dresden (1987), pp. 200-203.
8. N. P. Morozov and D. I. Tetel'baum, Fiz. Tekh. Poluprovod., 17, No. 5, 838-843 (1983).
9. P. Bellon, J. P. Chevalier, G. Martin, et al., Inst. Phys. Conf., No. 87, 309-314 (1987).
10. G. Vitali, M. Kalitzova, N. Pashov, et al., Appl. Phys., A45, No. 2, 133-135 (1988).
11. A. V. Chernyaev, Ion-Implantation Method in the Technology of Gallium Arsenide Devices and ICs [in Russian], Moscow (1990).