Diffusion and drift of Si dopants in δ-doped n-type $Al_xGa_{1-x}As$

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The study of diffusion and drift of Si in $Al_xGa_{1-x}As$ by means of capacitance-voltage measurements reveals that low substrate temperatures during growth by molecular beam epitaxy are required to achieve δ-function-like doping profiles. The diffusion coefficient of Si in $Al_{0.3}Ga_{0.7}As$ is determined. We further show theoretically that the random Poisson distribution (usually assumed for dopant distributions in semiconductors) should be modified at high dopant concentrations due to repulsive interactions of impurities.

Semiconductors in which dopants are spatially confined to a thin, highly doped region can be grown by molecular beam epitaxy (MBE) by evaporation of dopants on the nongrowing crystal surface.[1-3] The thickness of the doped region has been shown to be on the order of few lattice constants in Si-doped GaAs.[1] High free-carrier concentrations[2,3] of 2×10^{13} cm^{-2} have been achieved. Spatial confinement of Si dopants in $Al_xGa_{1-x}As$ and selectively doped $Al_xGa_{1-x}As$/GaAs heterostructures is desirable due to improved transport characteristics of heterostructures which include enhanced concentrations[4] as well as the minimization of remote ionized impurity scattering[5] in selectively δ-doped heterostructures.

This letter assesses the crystal growth conditions under which δ-function-like doping profiles can be attained in $Al_xGa_{1-x}As$. Employment of capacitance-voltage measurements and rapid thermal annealing are used to determine the diffusion coefficient of Si in $Al_xGa_{1-x}As$. We estimate the importance of drift, i.e., the movement of impurities in the electric field of vicinal impurities. We further show theoretically that the random Poisson distribution should be modified at high dopant concentrations due to repulsive Coulomb interactions of impurities.

The $Al_{0.3}Ga_{0.7}As$ epitaxial layers used for the present study were grown by MBE in a Varian Gen II system at temperatures ranging from 500 to 700 °C. The samples grown at 500 °C were cleaved into several pieces and thermally annealed for 5 s at temperatures ranging from 600 to 1000 °C. Further experimental details were reported previously.[1,2,4]

Capacitance-voltage (C-V) profiles of Si δ-doped $Al_{0.3}Ga_{0.7}As$ are shown in Fig. 1. The profile of the sample grown at 500 °C exhibits a peak with full width of 51 Å at a depth of 990 Å. However, as the substrate temperature is increased to 600 and 700 °C significant broadening of the profiles is observed. The broad profiles elucidate that smearing of dopants over more than 100 Å occurs if δ-doped $Al_xGa_{1-x}As$ is grown at elevated substrate temperatures.

It is currently assumed that the growth of high quality $Al_xGa_{1-x}As$ by MBE requires high substrate temperatures such as 600–650 °C. However, an improvement in source purity as well as in residual pressure in the MBE system may extend the range of tolerable growth temperatures. The photoluminescence spectrum of undoped $Al_{0.34}Ga_{0.66}As$ depicted in Fig. 2 has indeed the typical features of high quality material such as strong bound exciton intensity, clearly resolved transitions, and narrow photoluminescence linewidth. Thus, $Al_xGa_{1-x}As$ of good crystalline perfection can be obtained at low growth temperatures which in turn are required for the spatial localization of Si dopants.

The C-V profiles of δ-doped $Al_xGa_{1-x}As$ rapidly thermally annealed at different temperatures for 5 s are depicted in Fig. 3. A systematic decrease in the peak concentration as well as an increase in width is observed with increasing annealing temperature. The width (2σ) of the C-V profiles allows us to determine the approximate diffusion length associated with each annealing temperature using the relation

$$\sigma^2 = \sigma_{\rm diff}^2 + \sigma_i^2, \tag{1}$$

where σ_i represents the half width at half maximum of the C-V profile in the absence of diffusion ($\sigma_i \approx 25$ Å) and $\sigma_{\rm diff}$ is the diffusion-induced broadening of the C-V profile.

Diffusion in an initially δ-function-like dopant profile located at $z = 0$ results in a Gaussian dopant distribution with

$$N_D(z) = \frac{N_D^{2D}}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{z}{\sigma}\right)^2\right]. \tag{2}$$

The diffusion length is defined as $L_D = \sqrt{D\tau}$ and is related to the standard deviation of the Gaussian distribution by

$$L_D = \sqrt{D\tau} = \sigma/\sqrt{2}, \tag{3}$$

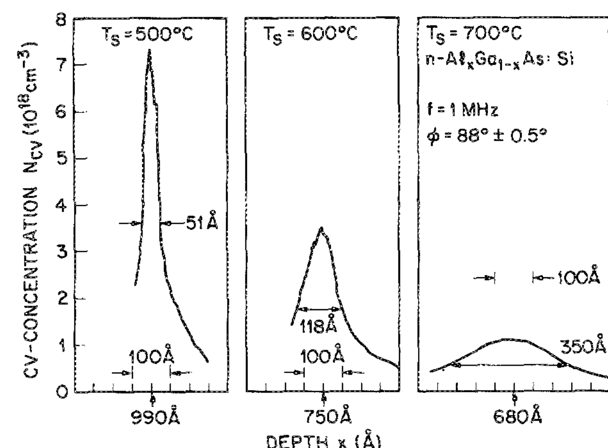

FIG. 1. C-V profiles measured at 300 K of δ-doped $Al_xGa_{1-x}As$ grown at substrate temperatures of 500, 600, and 700 °C.

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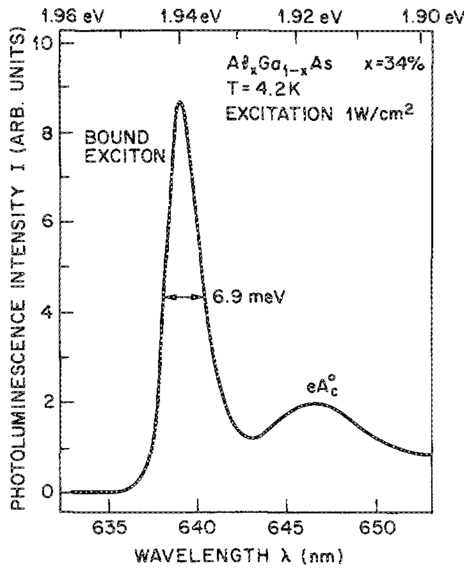

FIG. 2. Low-temperature photoluminescence spectrum of undoped $Al_{0.34}Ga_{0.66}As$ grown by MBE at a substrate temperature of 500 °C. The transitions are attributed to the bound exciton and a C-acceptor related transition.

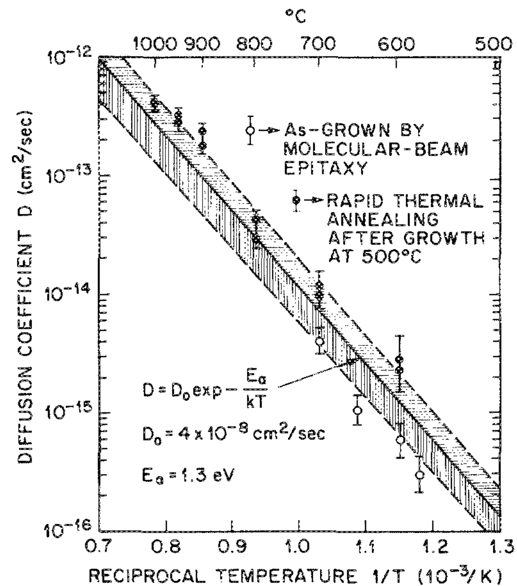

FIG. 4. Diffusion coefficient of Si in $Al_xGa_{1-x}As$ vs reciprocal temperature.

where τ is the time the sample is subjected to annealing. The diffusion coefficient of Si in $Al_xGa_{1-x}As$ is shown in Fig. 4. The experimental points are described best by an activation energy of $E_a = 1.3$ eV and a $D_0 = 4\times 10^{-8}$ cm²/s.

The presence of relatively high electric fields in δ-doped structures raises the question if the drift of ionized dopants is significant. Using the Einstein relation, the drift length of an ionized impurity atom within a homogeneous electric field F is given by

$$L_{\text{drift}} = D(e/kT)F\tau, \quad (4)$$

where e is the elementary charge and kT is the thermal energy. The electric field caused by the sheet of impurities is given by $F = eN_D^{2D}/2\epsilon$. The comparison of Eqs. (3) and (4) shows that short annealing times and low temperatures make diffusion the prevailing process in the redistribution of Si dopants. However, using the diffusion coefficient displayed in Fig. 4, drift is found to dominate at temperatures $T > 850$ °C for $\tau = 5$ s. Inspection of Fig. 4 in fact reveals that the diffusion coefficient at $T = 900$ °C ($D = 2\times 10^{-13}$ cm²/s) is surprisingly high as compared to the $T = 800$ °C ($D = 3\times 10^{-14}$ cm²/s) data point, which further indicates the importance of drift. At $T > 900$ °C dopants have spread out over distances $\gg 100$ Å such that the electric field decreases and drift becomes again less important.

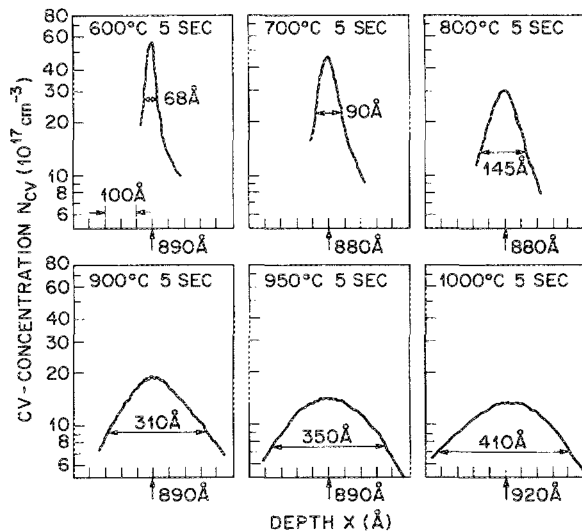

FIG. 3. C-V profiles of δ-doped $Al_xGa_{1-x}As$ annealed at different temperatures for 5 s.

In the following we will show that the repulsive Coulomb interaction can lead to correlation effects and to a deviation from the generally assumed Poisson distribution of dopants in highly doped semiconductors. If a homogeneously doped semiconductor has an uncorrelated dopant distribution with density N_D, the probability of finding A dopants within a volume V is given by the Poisson distribution:

$$p(A) = (N^A/A!)e^{-N}, \quad (5)$$

where $N = N_D$ is the average number of dopants within the volume V. For large N the Poisson distribution can be approximated by a Gaussian distribution with variance $\sigma^2 = N$ and expectation value N:

$$p(A) = \frac{1}{\sqrt{2\pi N}} \exp\left[-\frac{1}{2}\left(\frac{A-N}{\sqrt{N}}\right)^2\right]. \quad (6)$$

This distribution is shown in Fig. 5 by the solid curve for $N = 100$. The exponential term of the Gaussian distribution would correspond to the entropy term $\exp(TS/kT) = \exp(S/k)$ in a calculation based on statistical mechanics.[6]

The potential energy of repulsive donor ions of charge e is given by

$$E = \frac{1}{2}\sum_{i\neq j}\frac{e^2}{4\pi\epsilon r_{ij}}. \quad (7)$$

This energy is reminiscent of the Madelung energy in ionic

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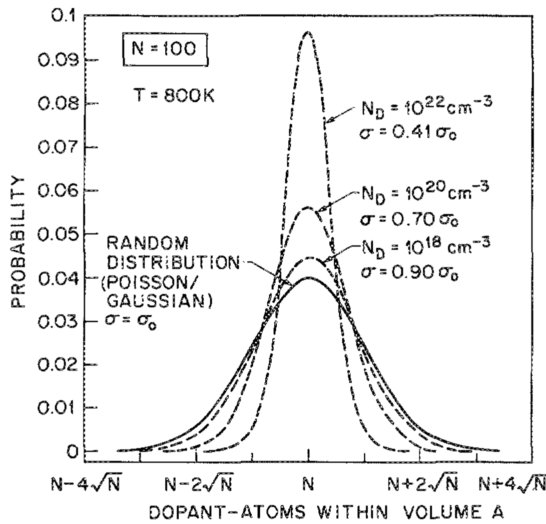

FIG. 5. Poisson distribution (solid line) of dopants in a semiconductor volume which contains an average of 100 dopant ions. Also shown are distributions (dashed lines) which deviate from the Poisson distribution due to Coulomb interaction of dopants at high concentrations. As a result the standard deviations σ of the new distributions decrease with increasing doping concentration.

crystals. The potential energy is minimized, if dopants are ordered in a face-centered-cubic lattice. For simplicity we assume that dopants are rather in a simple cubic lattice with the distance between dopants being $d = N_D^{-1/3}$. While the volume of an ordered impurity lattice contains N ions, different volumes may contain $N \pm \sqrt{N}$ ions for a random distribution. The mean distance then changes by

$$\sigma_d = \pm \tfrac{1}{3} N^{-5/6} V^{1/3}. \tag{8}$$

The introduction of the dimensionless parameter

$$\lambda = (A - N)/\sqrt{N} \tag{9}$$

allows one to change continuously from the ordered ($\lambda = 0$) to the random ($\lambda = 1$) distribution of dopant ions. The relative displacement is then given by

$$\sigma_d / d = \pm (1/3) \lambda^2 N^{-1/2}. \tag{10}$$

If a dopant atom is displaced by σ_d in the directions of the Cartesian coordinates, the mean increase of electrostatic energy (only next neighbors considered) is given by

$$\sigma_{E,1} = 3 \frac{e^2}{4\pi\epsilon} \frac{1}{d} \left(\frac{\sigma_d}{d} \right)^2. \tag{11}$$

The total increase of potential energy within the volume V due to an ordered-to-random transition of the impurity distribution is then given by

$$\sigma_{E,N} = (e^2/12\pi\epsilon) N_D^{1/3} \lambda^2. \tag{12}$$

Different dopant configurations thus correspond to different energies. Under conditions close to thermal equilibrium the configurations can be assumed to be distributed according to a Boltzmann distribution:

$$p(A) \sim \exp[-\sigma_E(A)/kT]. \tag{13}$$

The Boltzmann distribution changes the random distribution in terms of decreasing the probability of configurations far away from the average configuration ($A = N$). Combination of the Boltzmann distribution with the entropy factor of the Gaussian distribution yields after renormalization:

$$p(A) = \frac{1}{\sqrt{2\pi N}} \left(1 + \frac{e^2 N_D^{1/3}}{6\pi\epsilon kT} \right)^{1/2} \times \exp\left[-\frac{(A-N)^2}{2N} \left(1 + \frac{e^2 N_D^{1/3}}{6\pi\epsilon kT} \right) \right]. \tag{14}$$

For dilute doping concentrations ($N_D \leqslant 10^{18}$ cm^{-3}) the potential energy does not change the random distribution (solid line in Fig. 5). However, at high doping concentration significant deviations from the random Poisson distribution are expected. Note that screening is of minor influence, since the Thomas–Fermi screening length exceeds the interparticle distance at high doping concentrations. Semiconductors with nonrandom dopant distributions should exhibit new transport properties due to modifications of ionized impurity scattering as recently pointed out by Levi *et al.*[7] Such nonrandom dopant distributions were recently observed by x-ray diffraction: Headrick *et al.*[8] found B to be ordered in a two-dimensional, hexagonal structure in Si grown along the ⟨111⟩ direction.

As shown earlier the relative importance of drift and diffusion depends on the annealing conditions [see Eqs. (4) and (5)]. Random and nonrandom dopant distributions should therefore be possible under appropriate annealing or growth conditions.

In conclusion, the study of diffusion and drift in δ-doped $Al_xGa_{1-x}As$ reveals that low substrate temperatures are required during crystal growth by MBE to achieve spacially confined dopant distributions. The diffusion coefficient of Si in $Al_xGa_{1-x}As$ is determined. It is further shown theoretically that the random Poisson distribution should be modified at high doping concentrations due to Coulomb correlation effects.

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