COMPUTER SIMULATION OF THE IMPURITY DISTRIBUTION OVER THE THICKNESS OF A FILM DURING GROWTH OUT OF THE GAS PHASE

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The distribution of impurities over the thickness of a film is studied by computer simulation of the growth of the semiconducting film, taking into account attachment, detachment, reevaporation, and volume diffusion of atoms.

The distribution of impurities over the thickness of a film and in the transitional layer at the film—substrate boundary determines the electrophysical properties of devices, so that it is important to obtain information on profiles of impurity distributions. In most cases, the process responsible for the formation of profiles of foreign atoms is capture of atoms out of the gas phase [1] and diffusion out of the substrate [2]; the expected impurity distribution is found by solving the equation of diffusion with the appropriate boundary conditions [1-4]. Since in the process of diffusion, atoms can be captured by different defects with probability A, the redistribution of impurities is described by the equation [4]

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - AC. \tag{1}$$

For a well-defined value of the parameter A, the experimental and computed profiles of the doping of the film practically coincide. However, this analysis is based on an existing experimental profile, the value of A for which it coincides with the computed profile is determined, and conclusions are drawn concerning the nature of the traps.

The presently widely used methods of computer simulation of different processes [5, 6] yield information on the formation of the doping profile with condensation of atoms. Depending on the local configuration of atoms in the region of condensation, an impurity atom may appear to be in place or undergo a number of diffusion jumps over the growth time. The profiles of the distribution of foreign atoms obtained with simulation will depend on how completely the specific factors determining the growth of the film are taken into account and not on the values of the free parameter A in Eq. (1). In this paper, we study the formation of impurity profiles under different conditions by the method of computer simulation of the process of film growth.

To study the impurity distribution, we modeled the volume of a regular diamond-type crystalline lattice by a column that is 150 atomic layers high and has a base area of $n = 3 \times 6$ lattice points, oriented along the (111) plane. In studying the behavior of one type of impurity, the lower 15 layers initially described the structure of the substrate and the remaining 135 layers were empty. The height of the column, the number of layers in it, and the type of atoms at each node were stored in computer memory. We denoted the nodes containing atoms of the principal substance, impurity atoms, and vacancies as types 1, 2, and 3, respectively.

In obtaining the profile of the distribution of foreign atoms entering from the gas phase, it was assumed that the substrate initially contained vacancies, but not impurity atoms. To construct profiles of the densities of atoms penetrating into the film from the substrate, different contents of impurity atoms were fixed in the substrate. Both the vacancies and the impurity atoms were distributed in the substrate using a subroutine for generating pseudorandom numbers. The possibility of vacancy formation during the growth process was included.

For a flux density of atoms I, the number of atoms occurring in the adsorption position at a given point on the surface per unit time N_{ads} equals I/n_0, where n_0 is the reticular den-

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sity in the growth plane, while the time interval between two successive strikes of an atom at a given point is $t_0 = n_0/I$. Over this time, the adsorbed atom can be reevaporated from the surface or can remain in place, i.e., attached, and over the same period of time a surface atom can separate from the surface or remain in position. For this reason, we analyzed an identical number of detachments and reevaporations in the equilibrium state and for a relative oversaturation $\sigma = I/I_{eq}$, we performed $(\sigma + 1)$ analyses of reevaporations per detachment, and the duration of a single machine cycle equals $(\sigma/(\sigma + 1))t_0$. The rate of growth v, defined as the number of attaching atoms N_1 per N cycles, if $W = N_1/N$, equals

$$v = W\frac{\sigma+1}{\sigma}N_{\text{ads}}. \tag{2}$$

The number of diffusion jumps per unit time $\Gamma = \nu\exp\left(-\frac{E_D}{kT}\right)$, where E_D is the activation energy for diffusion, k is Boltzmann's constant, T is the temperature, and ν is the frequency of oscillations of an atom, is calculated from the coefficient of diffusion D. Taking into account the fact that the coefficient of diffusion $D = \frac{1}{6}\nu d^2\exp\left(-\frac{E_D}{kT}\right)$, we obtain $\Gamma = 6D/d^2$, where d is the length of a jump in a given direction. Over a time t_0, an atom can undergo Γt_0 jumps. If the volume being simulated initially contained N_0 atoms, then over a time t_0, it is necessary to simulate $N_0\Gamma t_0$ diffusion jumps per attachment. The number of atoms in the volume being simulated will increase during the growth process and then, over a time t_0, after N_1 atoms are attached, it is necessary to analyze $N_1\Gamma t_0$ more jumps. In analyzing diffusion relative to the plane in which the diffusing atom is located, we calculated the gradient of the concentrations $\nabla C = \Delta N_2/\Delta x$, where ΔN_2 is the number of impurity atoms in a well-defined number of layers Δx. The probabilities for a transition from region 1 into region 2 and back again were proportional to $K_1 = \nabla C_1/\nabla C_2$, $K_2 = \nabla C_2/\nabla C_1$; we assume that Δx equals 10 layers.

It was assumed that the probability of diffusion exchange of an atom of the i-th type, located at a given lattice point, with atoms of type j, located in a neighboring lattice point, is proportional to the frequency of oscillations of the i-th atom and depends exponentially on the exchange activation energy $\exp(-E_{ij}/kT)$ and inversely proportional to the square of the distance between these atoms. The expression for the exchange activation energy consists of 1, 2, or 3 terms: $E_{ij} = E_0 + \Delta Q + \Delta E$, where E_0 is the energy of activation of self-diffusion along vacancies; ΔQ is the change in the activation energy accompanying the exchange of an impurity atom with a vacancy; ΔE is the additional work expended on lattice deformation accompanying atom–atom exchange compared with atom–vacancy exchange as a function of type i and j nodes.

The highest exchange probability will occur for an atom of the principal substance with a vacancy situated at the nearest interatomic distance $d_{\min}$ in the given structure. We shall take it as equal to 1 and we shall express the remaining probabilities in terms of it, denoting them by ψ_{ij}, then $\psi_{13} = \psi_{31} = 1$; $\psi_{12} = \alpha f/\chi$; $\psi_{21} = \alpha f\chi$; $\psi_{23} = \chi\delta f$; $\psi_{32} = \delta f/\chi$, where $\chi = \nu_2/\nu_1 = \theta_2^D/\theta_1^D$ is the ratio of the characteristic Debye temperatures; $\delta = \exp(\Delta Q/kT)$; $f = d_{\min}^2/d_{ij}^2$; $\alpha = \exp(-\Delta E/kT)$.

The probabilities of diffusion exchanges were normalized so that there would be only one exchange within the time interval $\Delta\tau$.

For growth on the (111) plane in the 111 direction (Fig. 1), diffusion can occur into 16 nodes. However, to accelerate the calculation, diffusion jumps in the plane of growth were not analyzed and, in addition, instead of analyzing the remaining 10 possible exchanges (for an atom in an even layer in the four nearest nodes (4, 5, 6, 0') and in six locations in the upper layer (13, 14, 15, 16, 17, and 18); for an atom in an odd layer likewise in four nearest nodes (0, 4, 5, 6) and in six locations in the lower layer (7, 8, 9, 10, 11, and 12)), diffusion was analyzed only into two nodes out of the six nodes of the second coordination sphere, but the probability of such exchange was assumed to be three times higher.

The normalization condition has the form

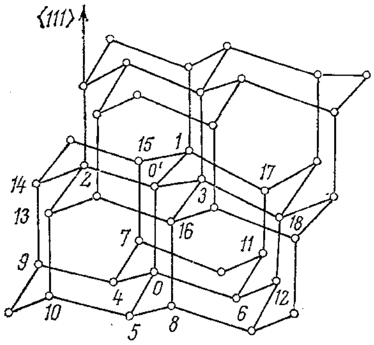

Fig. 1

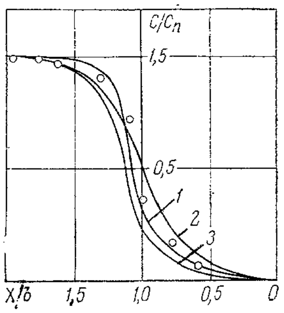

Fig. 2

Fig. 1. Diagram of distribution of atoms in the diamond lattice.

Fig. 2. Profiles of the distribution of phosphorus, migrating from substrates into epitaxial layers of silicon: 1) distribution obtained with the help of simulation; 2, 3) calculation according to (9) from [4] with the values A = 0 and $1.25\cdot10^{-3}$ $\sec^{-1}$.

$$\left[K_1 \sum_{m=1}^{3} (\psi_{ij})_m + K_2 \sum_{m=4}^{6} (\psi_{ij})_m\right] \Delta\tau = 1. \tag{3}$$

The range of possible events is divided into the number of subintervals, proportional to the number of predetermined locations for the transition, as in [6]. At the end of the calculation, the principal characteristics of the growth process [6] and the number of impurity atoms in each layer were printed out, which permits constructing the profile of the impurity distribution over the thickness.

The profiles of the phosphorus distribution in silicon, obtained by simulating diffusion of the impurity from the substrate (curve 1) and the profiles calculated using Eq. (9) from [4] for different values of the parameters A in the film (curves 2 and 3) are compared in Fig. 2. The origin of coordinates is located on the surface of the film, x/b = 1 corresponds to the film—substrate boundary, where b is the film thickness. In performing the calculation using Eq. (9) in [4], we used the experimental values of the velocity v = 0.3 μm/sec, time t = 20 sec, film thickness b = 6 μm, and growth temperature T = 1500°K from [7]. The experimental points are shown in the figure. Since in [7] the flux density of atoms is not indicated, we set it equal to $2\cdot10^9$ atoms/cm²·sec because the same rate of growth as in [7] is obtained in the simulation method with this flux density. Using the data in [8] on the diffusion of phosphorus into silicon, we estimated $\delta = 10^4$, $a = 2\cdot10^{-2}$, $\chi = 1, 2$. The values of the remaining parameters of the simulation were taken from [6].

Curves 1 and 3 do not pass through the point $C_{\text{film}}/C_{\text{substrate}} = 0.5$ at x = b, which indicates the influence of structural defects on the diffusion of impurities. Since the form of the computed curve (1) is close to the computed curve (3), we can say that the configuration of atoms arising in the growth being modeled includes defects that capture impurity atoms with probability A equal to $1.25\cdot10^{-3}$ $\sec^{-1}$.

In simulating the capture of foreign atoms out of the gas phase during the growth process, we obtained a temperature dependence of the penetration depth and of the transport coefficient and defectiveness of the film and of the substrate that qualitatively coincided with the experimental dependences. The penetration depth of the impurity increases with increasing temperature with constant impurity concentration in the gas phase. An increase in the concentration in the gas phase increases capture of impurities and gives rise to a large diffusion depth. Figure 3 shows the dependence of the depth of penetration of the impurity atoms into the substrate for films with identical thickness on the flux density of silicon atoms for two values of the phosphorus concentration in the gas phase. Curve 2 was obtained for a concentration that is two times higher than the concentration for curve 1. The high flux gives rise to rapid growth. In films with identical thickness, obtained for different velocities of growth, the depth of penetration of impurity atoms will be greater in films that were grown more slowly due to the longer diffusion time at high temperature.

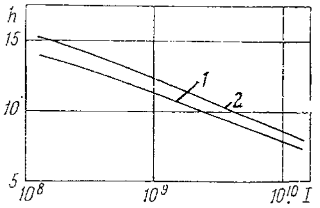

Fig. 3

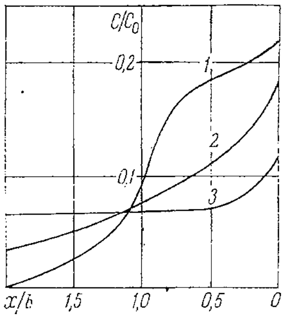

Fig. 4

Fig. 3. Dependence of the maximum depth of penetration of phosphorus into the substrate on the flux of atoms with a phosphorus concentration of 0.1% (1) and 0.2% (2). h is the number of atomic layers and I is in atoms/$\text{cm}^2 \cdot \text{sec}$.

Fig. 4. The diffusion distribution of phosphorus entering from the gas phase into epitaxial layers of silicon with: 1) D/bv = 0.5; 2) 1; 3) 2.

Simulation of the formation of the diffusion profile of the impurity, entering into the film and the substrate out of the gas phase during growth, permits following clearly the influence of the relation between the velocity of growth and the velocity of diffusion on the character of the impurity distribution, i.e., it permits analyzing the role of the basic parameters entering into the corresponding solutions of the diffusion equations. In the simulation, this is achieved by changing the relation between the numbers of analyses of attachments and diffusion exchanges. The number of diffusion exchanges is constant for a given temperature, while the growth velocity can be changed.

The criterion for stationarity in the analytic description of the growth process is the parameter D/bv; for $D/bv < 1$, the growth is nonstationary. Replacing D by the number of jumps and expressing the growth velocity (2) and the thickness $b = N_1/n$ in the SI system, we find that in the computer experiment, the quantity $D/bv = 1$ corresponds to $\Gamma[6N_{ads}Wb(1 + I_{eq}/n_0N_{ads})]^{-1} = 1$. At T = 1500°K, the growth of silicon will be nonstationary for $W = 0.8$, $b = 12$ layers with $\Gamma/N_{ads} < 2$.

Profiles of the distribution of phosphorus captured during the growth of silicon films with different velocities at T = 1500°K are shown in Fig. 4. The concentration of phosphorus in the solid phase and the distance from the film–substrate boundary in fractions of the film thickness are plotted along the coordinate axes. Curve 1 corresponds to slow, compared to the growth velocity, diffusion $\Gamma/N_{ads} = 1$, $D/bv < 1$, i.e., impurity atoms diffuse into the substrate practically out of a layer with constant concentration, which is formed with rapid growth of the film. Curve 2 was obtained for a lower growth velocity $\Gamma/N_{ads} = 2$, $D/bv = 1$. Curve 3 was obtained for $\Gamma/N_{ads} = 4$. $D/bv = 2$. This is the case of stationary growth; the impurity has time to diffuse deeply and a practically equilibrium profile is established. The concentration of impurity atoms in the flux was assumed to be constant in all cases. The number of foreign atoms, captured during growth, defined as the area under the curve (Fig. 4), is the same in all cases, if the nonequilibrium surface layer with thickness 0.2b is omitted. The curve, constructed from the solution of the diffusion equation (8) in [4] with D/bv = 0.5 coincides completely with curve 1, while curve 3 corresponds to the stationary solution of Eq. (1).

Thus simulation of diffusion exchanges in the volume of a film confirmed that the formation of the profile of the distribution of impurities entering from the substrate depends on the degree of perfection of the structure of the transitional layer, while the nature of the distribution of impurity atoms captured out of the gas phase depends on the growth velocity and growth time.

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