Journal of Engineering Physics and Thermophysics, Vol. 71, No. 2, 1998

NONLINEAR DISTRIBUTION MODEL OF IONS IMPLANTED AT HIGH DOSES

A. L. Danilyuk

UDC 621.382

A nonlinear distribution model of ions implanted at high doses is developed with allowance for sputtering, volume growth of a target, and retardation by interstitial atoms.

High-dose implantation models based on distribution functions [1-4] are rather simple. However, their use necessitates consideration of the dependences of parameters of these functions on the concentration of implanted ions, which are determined by many factors and are a priori unknown. Therefore, any attempts to allow for this change by introducing different intuitive assumptions should be recognized as incorrect since the reasoning behind those assumptions is unclear.

The model suggested allows for target sputtering, its volume growth, and retardation by interstitial atoms. It does not need the introduction of any assumptions on changing the distribution function with an increase in dose. The model is based on two assumptions. The first assumption implies that an ion profile at a low dose in a pure substance of a target and in a binary substance consisting of target atoms and implanted ions at their stoichiometric concentration is described by the same type of this function. The second assumption concerns the type of the distribution function valid at low doses in these substances. At present, such functions are well known since they have been established by numerous theoretical and experimental studies. They include symmetrical and asymmetrical Gauss distributions, the Pearson distribution, etc. [5, 6]. The model is valid in the dose range when the distribution profile has no plateau and the sputtering coefficient is $Y < 1$.

The model is based on the following principle. Ion implantation is considered at low doses ΔD ($10^{14}-10^{15}$ cm^{-2}) when for binary targets the moments of a distribution function can be calculated by known functions or determined from tables. In so doing, sputtering, volume growth of a target, and additional retardation by implanted atoms are taken into consideration at each step. The sputtering and volume growth are accounted for by a shift of the coordinates, while additional retardation dependent on the magnitude and the gradient of the concentration of implanted atoms by the modified method of dose correction [7]. A profile of low-dose distribution $\Delta N(x, \Delta D)$ is built by dividing the profile of implanted atoms $N(x, D)$ into narrow layers with thickness Δx_j. The concentration of the implanted atoms is each layer is assumed to be constant. Then distribution functions are written for a low dose in materials that have characteristics of the layers under consideration (i.e., at definite concentrations of implanted atoms and target atoms). Next, using the dose-correction method, a distribution function is built for a newly implanted low dose of ions for each jth narrow layer with due regard for the presence of $j-1$ layers. These steps are repeated until a complete collection of the required dose is reached.

Let us consider the constitution of the profile of implanted ions. For this, we divide the profile $N(x, D)$ into layers with thickness Δx_j and consider low-dose implantation ΔD. Assume that $x_1, x_2, \dots x_n$ are the layer coordinates; $f_1, f_2, \dots, f_n$ are the distribution functions for newly implanted ions with respect to depth in these layers. When constructing the functions $f_1, f_2, \dots, f_n$, the layers are considered independently of each other and are characterized by their definite concentrations of the implanted atoms and target atoms. The distribution function for the kth layer is written as $f_k\ (x, m_{1k}, m_{2k}, \dots, m_{mk})$, where $m_{1k}, m_{2k}, \dots, m_{mk}$ are the moments of the ion distribution function in a material that has characteristics of the considered layer k. The moments $m_{1k}, m_{2k}, \dots, m_{mk}$ are determined by the concentrations of implanted atoms and target atoms in the kth layer. Implantation

---

Belarusian State University of Information Science and Radioelectronics, Minsk, Belarus. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 71, No. 2, pp. 277-281, March-April, 1998. Original article submitted November 22, 1996.

of the dose ΔD occurs in narrow layers arranged one after another. A profile of the distribution $\Delta N\ (x, \Delta D)$ is built, according to the dose-correction method, by shifting the coordinates of the functions $f_1, f_2, \ldots, f_n$ in each layer by values of the equivalent depths $w_1, w_2, \ldots, w_n$. The values of $w_1, w_2, \ldots, w_n$ determine coordinate shifts under the assumption that each previous layer possesses the same characteristics as the following layer.

The value of w_k in the case of narrow layers (the coordinate of the origin of the first layer is taken as zero) is determined by the expression [7]

$$\sum_{j=1}^{k-1} \Delta D_j = \Delta D \sum_{0}^{w_k} f\,(z, m_{1k}, m_{2k}, \ldots, m_{mk})\, dz\,, \tag{1}$$

where

$$\Delta D_1 = \Delta D \int_0^{x_1} f_1\,(x, m_{11}, m_{21}, \ldots, m_{m1})\, dx \approx \Delta D f_1\,(x, m_{11}, m_{21}, \ldots, m_{m1})\, \Delta x_1\,;$$

$$\Delta D_2 = \Delta D \int_{x_1}^{x_2} f_2\,(x + w_2 - x_2\,,\ m_{12}, m_{22}, \ldots, m_{m2})\, dx \approx$$

$$\approx \Delta D f_2\,(x + w_2 - x_2\,,\ m_{12}, m_{22}, \ldots, m_{m2})\, \Delta x_2\,;$$

$$\Delta D_j = \Delta D \int_{x_{j-1}}^{x_j} f_j\,(x + w_j - x_j\,,\ m_{1j}, m_{2j}, \ldots, m_{mj})\, dx \approx$$

$$\approx \Delta D f_j\,(x + w_j - x_j\,,\ m_{1j}, m_{2j}, \ldots, m_{mj})\, \Delta x_j\,. \tag{2}$$

Performing summation over (2), we arrive at

$$\sum_{j=1}^{k-1} \Delta D_j = \sum_{j=1}^{k-1} \Delta D f_j\,(x + w_j - x_j\,,\ m_{1j}, m_{2j}, \ldots, m_{mj})\, \Delta x_j\,. \tag{3}$$

Letting Δx_j tend to zero and comparing (1) and (3), we obtain an equation for determining the function of coordinate shift $w(x)$ upon implantation of the dose ΔD:

$$\int_0^x f\,[w\,(x), m_1\,(N), m_2\,(N), \ldots, m_m\,(N)\,]\, dx =$$

$$= \int_0^{w(x)} f\,[z, m_1\,(N), m_2\,(N), \ldots, m_m\,(N)\,]\, dz\,. \tag{4}$$

In Eq. (4), the moments $m_1(N), m_2(N), \ldots, m_m(N)$ are independent of the parameter z.

Allowance for the processes of sputtering and volume growth leads to a shift of the coordinates under implantation conditions. A change in the x coordinate will be written in the form

$$\Delta x = \Omega \int_x^{\infty} \Delta N\,(x)\, dx - Y\Delta D/(N_{m0} + N_0)\,. \tag{5}$$

Considering that $\Delta N(x) = \Delta D f[w, m_1(N), m_2(N), \ldots, m_m(N)\,]$ and letting ΔD tend to zero, after some transformations we obtain a system of differential equations

$$dN/dD = f\,(w, N)\,, \tag{6}$$

$$(dx/dD)/\Omega = 1 - \Omega_m Y\,[(1 + \Omega_m N_0)\,\Omega]^{-1} - \int_0^x f(w, N)\,dx\,, \tag{7}$$

where

$$f(w, N) = f\,[w(x), m_1(N), m_2(N), \ldots, m_n(N)]\,, \tag{8}$$

which, together with (4), allow calculation of a profile of the ion-implantation distribution in the considered model as a function of the dose.

Considering that in the present nodel the x coordinate is a function of the dose and that in Eq. (4) the moments are independent of the parameter z, we reduce the relations obtained to a system of ordinary differential equations. For this, we differentiate Eq. (4) with respect to x and q, and Eq. (7) – with respect to q.

After some transformations we arrive at the following system of equations:

$$dN/dq = (R_0/\Omega)\,f(w, N)\,, \tag{9}$$

$$dx/dq = \varphi R_0\,, \tag{10}$$

$$d\varphi/dq = -f(w, N)\,\varphi R_0\,, \tag{11}$$

$$dw/dq = \varphi R_0 - (R_0/\Omega)\int_0^w [\delta f(z, N)/\delta N]\,dz\,. \tag{12}$$

Here

$$\varphi = 1 - \Omega_m Y\,[(1 + \Omega_m N_0)\,\Omega]^{-1} - \int_0^x f(w, N)\,dx\,, \tag{13}$$

$$f(z, N) = f\,[z, m_1(N), m_2(N), \ldots, m_n(N)]\,, \tag{14}$$

If the distribution of ions implanted at low doses is modeled by the Gaussian function, then

$$f(y, N) = [\sqrt{2\pi}\,\Delta(N)]^{-1}\exp\left\{-[y - R(N)]^2/2\Delta^2(N)\right\}, \tag{15}$$

where $y = w$ or z. If this distribution is modeled by the Pearson IV function, then

$$f(y, N) = k\,[1 + (y/a)^2]^{-q}\exp[-\nu\arctan(y/a)]\,, \tag{16}$$

In (16), the Pearson IV distribution parameters k, a, q, ν depend on the concentration of implanted ions N. Relationships between them and mean projected range, straggling, asymmetry, and excess are given in [8].

For a binary material with constant concentrations of atoms N_m and ions N, we have [5]

$$R(N) = [(\Omega_0 N_m/R_0 + (\Omega_{0i}N/R_{0i})]^{-1}\,, \tag{17}$$

$$\begin{aligned}\Delta(N) = R(N)\,[(R_{0i}\,\Omega_0 N_m)\,(\Delta_0/R_0)^2/(R_0\Omega_{0i}N) + (\Delta_{0i}/R_{0i})^2]^{1/2} \times \\ \times\,[(R_{0i}\,\Omega_0 N_m)/(R_0\Omega_{0i}\,N) + 1]^{-1/2}.\end{aligned} \tag{18}$$

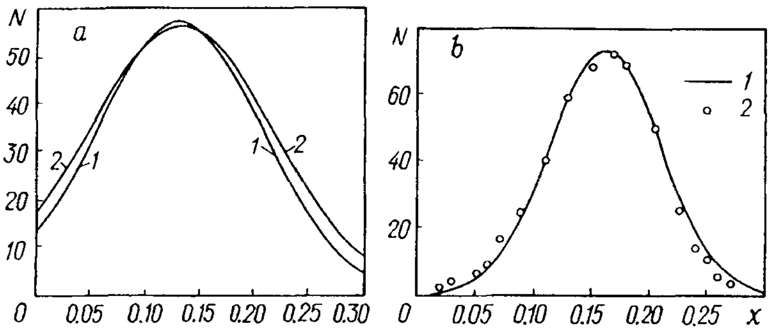

Fig. 1. Distribution of the implanted oxygen concentration N in aluminum (a) (energy of 60 keV, dose of $6 \cdot 10^{17}$ cm^{-2}) and silicon (b) (60 keV, $5 \cdot 10^{17}$ cm^{-2}) with respect to depth x; a: 1) calculation, 2) experiment [10], processing by the least-square method; b: 1) calculation, 2) experiment [9]. N, at. %; x, μm

Expressions (17), (18) are valid provided that the retardation capacities of the elements of the binary compound depend on energy in a similar manner [5].

An analysis of the equations obtained has shown that they correspond to the models [1-4] provided the influence of the retardation function $w(x)$ is neglected. Whence it follows that formation of the second phase in ion formation must be taken into consideration not only in the dependences of the moments of distribution functions but of the coordinate shift as well.

The system of equations (9)-(18) allows calculation of the distribution of implanted ions for high doses with an account of the limitations if the type of distribution function is specified for small doses in a binary material consisting of target atoms and implanted element atoms with the concentration of the latter ranging from stoichiometric to the initial one.

As an example, we have calculated profiles of the distribution of oxygen implanted into silicon at an energy of 60 keV and a dose of $5 \cdot 10^{17}$ cm^{-2} and into aluminum at an energy of 60 keV and a dose of $6 \cdot 10^{17}$ cm^{-2}. For the distribution function at low doses, we chose a symmetrical Gaussian distribution characterized by two moments, namely, the mean projected range R_0 and the root-mean-square range (straggling) Δ_0.

Calculation results were compared to experimental data. Experimental profiles of oxygen implanted into silicon (at an energy of 60 keV, dose $5 \cdot 10^{17}$ cm^{-2}, without annealing) were obtained from x-ray photoelectronic and infrared spectroscopic data of the samples subjected to layer-by-layer etching [9]. Profiles of oxygen distribution in aluminum were determined by the Rutherford back scattering (RBS) method [10]. Oxygen implantation into aluminum was carried out at an energy of 60 keV, dose of $6 \cdot 10^{17}$ cm^{-2}, and an ion current density of 3 μA/cm in order to avoid target heating. Results are given in Fig. 1, which shows quite satisfactory agreement.

The divergence between the calculated and experimental profiles of oxygen in aluminum is due, in our opinion, to the influence of the processes of diffusion and generation of defects, an account of which was not carried out in the present work. Note that this can be easily accomplished by adding them.

Thus, a nonlinear distribution model of ions implanted at high doses is developed which allows for target sputtering, its volume growth, and retardation by implanted atoms.

NOTATION

x, z, coordinates dependent on and independent of a dose, respectively; N, concentration of the implanted ions; $f(x, N)$, distribution function in a binary compound consisting of target atoms and ions of the implanted element with concentration N; $m_1(N)$, $m_2(N)$, ..., $m_m(N)$, moments of the distribution function dependent on the concentration of implanted ions for a binary component; Ω, volume per implanted ion; Ω_m, volume per target atom; Ω_{0i}, volume per atom in a substance consisting only of implanted ions (at their stoichiometric concentration); Y, coefficient of target sputtering; N_{m0}, atomic concentration of the target at $x = 0$; N_0, ion concentration at $x = 0$; N_m, atomic concentration of the target in the course of implantation; $q = \Omega D/R_0$, generalized (dimensionless) dose; $R(N)$, $\Delta(N)$, mean projected range and straggling for a binary compound consisting of target atoms and implanted atoms for different constant element concentrations N; R_{0i}, Δ_{0i}, mean projected range and straggling of ions in a substance consisting of implanted ions (at their stoichiometric concentration); R_0, Δ_0, mean projected range and straggling of ions in a pure material of the target; k, a, q, ν, parameters of the Pearson IV distribution.

REFERENCES

1. H. U. Joger, Phys. Stat. Sol., **A103**, K75-79 (1987).
2. H. U. Joger, Nucl. Ins. Meth. Phys. Res., **B65**, 67-72 (1992).
3. V. V. Titov, Zh. Tekh. Fiz., **49**, 844-847 (1979).
4. V. G. Abdrashitov and V. V. Ryzhov, Fiz. Khim. Obrab. Mater., No. 6, 14-18 (1990).
5. M. A. Kumakhov and F. F. Komarov, Energy Losses and Ion Ranges in Solids [in Russian], Minsk (1979).
6. F. F. Komarov, A. P. Novikov, and A. F. Burenkov, Ion Implantation [in Russian], Minsk (1994).
7. V. P. Sidorenko, N. V. Grudanov, V. E. Savitskii, V. B. Nevzorov, and V. I. Beregovoi, Izv. VUZov, Radioélektronika, **32**, 43-46 (1989).
8. A. F. Burenkov, F. F. Komarov, M. A. Kumakhov, and M. M. Temkin, Tables of the Parameters of Space Distribution of Ion-Implanted Impurities [in Russian], Minsk (1980).
9. V. A. Labunov and P. V. Protasevich, Nucl. Ins. Meth. Phys. Res., **B39**, 466-468 (1989).
10. A. L. Danilyuk, V. V. Uglov, and N. N. Cherenda, Izv. Belorus. Inzh. Akad., No. 1 (1), 59-62 (1996).