NONLINEAR DISTRIBUTION MODEL OF IONS IMPLANTED AT HIGH DOSES

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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 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 $AD (10^{14}-10^{15} \text{cm}^{-2})$ 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 $\Delta N(x, AD)$ is built by dividing the profile of implanted atoms $N(x, D)$ into narrow layers with thickness $\Delta x_j$. The concentration of the implanted atoms in 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 $j$th 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 $\Delta x_j$ and consider low-dose implantation $\Delta D$. Assume that $x_1, x_2, ..., x_n$ are the layer coordinates; $f_1, f_2, ..., f_n$ are the distribution functions for newly implanted ions with respect to depth in these layers. When constructing the functions $f_1, f_2, ..., f_n$, 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 $k$th layer is written as $f_k (x, m_{1k}, m_{2k}, ..., m_{nk})$, where $m_{1k}, m_{2k}, ..., m_{nk}$ are the moments of the ion distribution function in a material that has characteristics of the considered layer $k$. The moments $m_{1k}, m_{2k}, ..., m_{nk}$ are determined by the concentrations of implanted atoms and target atoms in the $k$th layer. Implantation...
of the dose $\Delta D$ 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]

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

where

\[
\Delta D_1 = \Delta D \int_0^{x_1} f_1(x, m_{11}, m_{21}, \ldots, m_{m1}) \, dx = \Delta D f_1(x, m_{11}, m_{21}, \ldots, m_{m1}) \Delta x_1;
\]
\[
\Delta D_2 = \Delta D \int_{x_1}^{x_2} f_2(x + w_2 - x_2, m_{12}, m_{22}, \ldots, m_{m2}) \, dx = \Delta D f_2(x + w_2 - x_2, m_{12}, m_{22}, \ldots, m_{m2}) \Delta x_2;
\]
\[
\Delta D_j = \Delta D \int_{x_{j-1}}^{x_j} f_j(x + w_j - x_j, m_{1j}, m_{2j}, \ldots, m_{mj}) \, dx = \Delta D f_j(x + w_j - x_j, m_{1j}, m_{2j}, \ldots, m_{mj}) \Delta x_j.
\]

Performing summation over (2), we arrive at

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

Letting $\Delta x_j$ 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 $\Delta D$:

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

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

\[
\Delta x = \int_0^\infty \Delta N(x) \, dx - Y\Delta D/(N_{m0} + N_0).
\]

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

\[
dN/dD = f(w, N),
\]