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MODEL OF LASER GETTERING OF FAST-DIFFUSING IMPURITIES

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A model of gettering of fast-diffusing impurities in silicon wafers has been proposed; this model makes it possible to determine efficient gettering regimes ensuring the production of high-quality silicon wafers with reproducible characteristics for using them in the technology of creation of very large-scale integrated circuits.

The technology of submicron integrated circuits (ICs) places heavy demands on different materials and primarily on silicon. A large role is played by the presence of point defects and contaminating impurities, such as copper, iron, nickel, chromium, sodium, and others, in it. This leads to a reduction in the yield of suitable ICs because of the uncontrolled process of defect formation in the region of active layers. The use of gettering methods (introduction of damage into the reverse side of the wafer by mechanical action, ion implantation, and pulsed laser radiation, or formation of an internal getter based on the use of the intrinsic oxygen) makes it possible to reduce the influence of these negative phenomena. These processes have a low controllability, however, and are inefficient and inadequately studied as applied to the technology of submicron ICs. The most promising is the method based on the use of continuous laser radiation. In this case, the gettering layer is created by the action of two factors: high thermal stresses at the liquid–solid phase boundary and the presence of the liquid phase itself in the region of treatment for a long period under the action of laser radiation. On the idle side of the wafer, we have tensile stresses, which is opposite to the Twyman effect related to the occurrence of stresses due to the mechanical disturbances of the crystal lattice [1]. An important feature of the method of laser gettering is the absence of the return flow of fast-diffusing impurities from the gettering layer into the wafer's volume in both the process itself and the subsequent high-temperature treatments.

To model the process of gettering we consider the basic phenomena accompanying this process. Treatment of the idle side of a wafer by continuous laser radiation with a power density of $5.5 \cdot 10^5$ W/cm^2 and a scanning step of 200 μm is accompanied by the occurrence of considerable thermal stresses in silicon. In subsequent long-duration, high-temperature action, the stresses relax to form dislocations and oxygen precipitates, which are traps for impurity atoms and point defects, in the silicon layer of thickness $h^* << h$. For the sake of simplicity, we will assume that the traps in the gettering layer and the fast-diffusing impurities across the wafer thickness are distributed uniformly and their concentrations N_{tr0} and N_i are respectively

$$N_{tr0} = N_{tr}(x, 0) , \tag{1}$$

$$N_{0i} = N_i(x, 0) , \quad i = 1, 2, ..., n . \tag{2}$$

Since the impurity atoms will first be captured by the traps at the gettering layer–substrate boundary, the concentration will decrease quickly in this region and, for $x = h^*$, will be equal to

$$N_i(h^*, t) = 0 . \tag{3}$$

The resulting concentration gradient of the impurity will contribute to its further diffusion from the wafer's volume into the gettering layer. In the region $h^* \le x \le h$, this process is described by the system of Fick's diffusion equations [2]

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$$\partial N_i / \partial t = D_i \partial^2 N_i / \partial x^2 , \quad i = 1, 2, ..., n . \tag{4}$$

The boundary condition for $x = h$ has the following form:

$$\partial N_i / \partial x \big|_{x=h} = 0 . \tag{5}$$

We place the origin of coordinates at the gettering layer–substrate boundary and guide the x axis toward the working surface of the wafer. Integrating expression (4), we obtain

$$N_i (x, t) = N_{0i} (4\pi D_i t)^{-1/2} \int_0^h \left\{ \exp [-(x - x')^2 / 4D_i t] - \exp [-(x + x')^2 / 4D_i t] \right\} dx' . \tag{6}$$

We introduce the following notation:

$$\alpha = x / [2 (D_i t)^{1/2}] , \quad \beta = (h - x) / [2 (D_i t)^{1/2}] , \quad \gamma = (h + x) / [2 (D_i t)^{1/2}] , \quad U = x - x' / [2 (D_i t)^{1/2}] .$$

Then expression (6) will take the form

$$N_i (x, t) = N_{0i} (\pi)^{-1/2} \int_{-\alpha}^{\alpha} \exp (-U)^2 \, dU + N_{0i} (\pi)^{-1/2} \int_0^{\beta} \exp (-U)^2 \, dU - N_{0i} (\pi)^{-1/2} \int_0^{\gamma} \exp (-U)^2 \, dU . \tag{7}$$

After the integration of expression (7), we obtain

$$N_i (x, t) = N_{0i} [\mathrm{erf}\, \alpha + 0.5 (\mathrm{erf}\, \beta - \mathrm{erf}\, \gamma)] . \tag{8}$$

Substituting the values of α, β, and γ into (8), we have

$$N_i (x, t) = N_{0i} \left\{ \mathrm{erf}\, x / [2 (D_i t)^{1/2}] + 0.5\, \mathrm{erf}\, (h - x) / [2 (D_i t)^{1/2}] - 0.5\, \mathrm{erf}\, (h + x) / [2 (D_i t)^{1/2}] \right\} . \tag{9}$$

Expression (9) describes the change in the concentration of the fast-diffusing impurity in the wafer's volume as a result of its diffusion into the gettering layer. The quality of epitaxial films and ICs largely depends on the state of the surface silicon layer on the working side of the wafer. Consequently, we must primarily achieve a decrease in N_i in it. Setting $x = h$ in (8), we obtain an expression describing the change in the surface concentration of the fast-diffusing impurity on the working side of the wafer in the process of gettering:

$$N_i (h, t) = N_{0i} \left\{ \mathrm{erf}\, [h (4D_i t)^{-1/2}] - 0.5\, \mathrm{erf}\, [h (D_i t)^{-1/2}] \right\} . \tag{10}$$

To calculate the temperature and the time necessary for the process of gettering we introduce the "gettering criterion," by which we will mean the process resulting in a decrease of two orders of magnitude in the initial concentration of the fast-diffusing impurity:

$$N_i (h, t) / N_{0i} \le 10^{-2} . \tag{11}$$

This condition means that virtually the entire contaminating impurity from the wafer's volume has passed into the gettering layer. The calculation carried out for copper impurity atoms according to expression (10) with account for the change in their diffusion coefficient as a function of the temperature

$$D = 4 \cdot 10^{-2} \exp (-1.0 / kT) \tag{12}$$

has shown (see Fig. 1) that it is expedient to carry out gettering at a temperature of 1100°C and a time of no shorter than 20 min. The use of lower temperatures does not lead to the total relaxation of thermal stresses to form dislocations in the gettering layer, which decreases the sink and the capture of the fast-diffusing impurities by it.

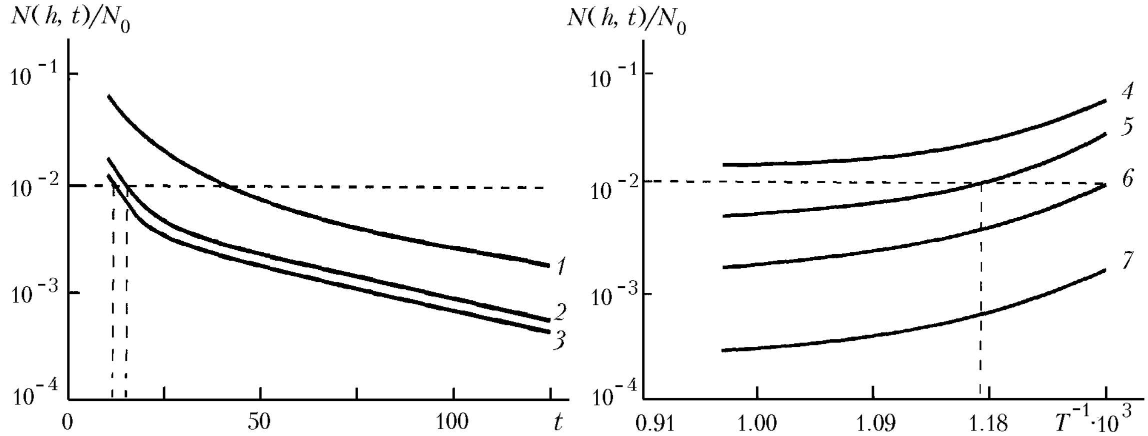

Fig. 1. "Gettering criterion" vs. time and inverse temperature of high-temperature treatment: 1) 1000, 2) 1100, and 3) 1200°C; 4) 10, 5) 20, 6) 40, and 7) 120 min.

Gettering proceeds as long as the condition

$$N_{ig} h^* \geq N_i (x, t)\, h\,. \tag{13}$$

is fulfilled. What this means is that the process of diffusion of the impurities into the gettering layer is limited by their initial concentration in the wafer and the capacity of the getter.

If we have

$$N_{0i} > N_{ig}^{\lim} h^* / h\,, \tag{14}$$

the process of gettering will not proceed.

We find the limiting surface concentration of fast-diffusing impurities that can be captured by the gettering layer. Since the sites of gettering in silicon are oxygen precipitates, each of which is capable of capturing $4 \cdot 10^9$ point defects and fast-diffusing impurities [3], the limiting surface concentration of the impurity captured by the gettering layer may attain $4 \cdot 10^{17}$ cm^{-2}.

The calculation carried out in accordance with expression (14) for a depth of the gettering layer of 10 μm and a thickness of the silicon wafer of 360 μm has shown that the limiting surface concentration of the impurity in the initial wafer having the possibility of diffusing to the gettering layer is $1.1 \cdot 10^{16}$ cm^{-2}. Investigation of the initial silicon wafers by the neutron-activation method has made it possible to establish that the basic contaminating impurities are sodium, copper, iron, nickel, and chromium, whose surface concentration is $5.5 \cdot 10^{13}$, $1.8 \cdot 10^{12}$, $3.6 \cdot 10^{12}$, $4.7 \cdot 10^{14}$, and $3.6 \cdot 10^{10}$ cm^{-2} respectively. What this means is that the gettering layer created with the use of continuous laser radiation is able to capture not only the impurities in the initial silicon wafers but also those introduced in subsequent long-duration, high-temperature operations.

Thus, the model proposed makes it possible to describe the process of laser gettering and to substantiate the parameters (temperature and time) necessary for the efficient diffusion of a contaminating impurity to the gettering layer, which enables one to produce high-quality initial silicon wafers, thus reducing the number of defects in the active regions of ICs.

NOTATION

D_i, coefficient of diffusion of an impurity of the ith type, cm^2·sec^{-1}; h, thickness of the silicon wafer, μm; h^*, thickness of the gettering layer, μm; k, Boltzmann constant, eV/°C; N_i, concentration of impurity atoms in the wafer, cm^{-2}; N_{0i}, concentration of impurity atoms or defects of the ith type in the wafer at t = 0; $N_{\rm tr}$, concentration of traps in the gettering layer; $N_{\rm tr0}$, concentration (density) of traps in the gettering layer at t = 0; N_{ig}, surface concentration of the fast-diffusing impurity captured by the getter; N_{ig}^{lim}, limiting concentration of the fast-diffusing impurity that can be captured by the gettering layer; n, number of types of fast-diffusing impurity atoms or other point defects; t, heat-treatment time, sec; T, temperature. Subscripts and superscripts: g, getter; i, type of impurity; tr, trap; lim; limiting.

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