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EFFECT OF CHARGED CLUSTERS ON THE DIFFUSION OF IMPURITY ATOMS IN SILICON CRYSTALS

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An equation of diffusion of impurity atoms in silicon crystals has been obtained, based on which the influence of charged clusters in a silicon crystal on the process of impurity transfer can be determined. It is shown that a characteristic feature of this effect is the appearance of an additional flux of impurity atoms, which is capable of leading to impurity segregation.

Keywords: *diffusion, segregation, cluster, impurity, silicon.*

Introduction. As is known, in the production of current superlarge integrated circuits wide use is made of low-energy high-dose implantation of ions in silicon plates in combination with their thermal treatment for annealing the defects formed during the incorporation of ions. In the process of annealing the ion-implanted silicon layers, diffusion redistribution of impurity atoms occurs in them. This means that the final distribution of impurity atoms in a silicon sublayer is determined as much by the implantation parameters as by the characteristics of the diffusion process. The use of ion implantation allows one to create doped silicon layers with the concentration of impurity atoms greatly exceeding the impurity solubility limit. Thermal annealing of such layers causes the clustering of impurity atoms [1]. The influence of the formation of neutral clusters in a silicon plate on the diffusion of impurity in it is expressed as the disengagement of part of the impurity atoms from the process of transfer. A change in the state of the defect subsystem of the crystal is also possible as a result of the absorption or generation of point defects in clustering. However, as was shown in [2, 3], in silicon layers doped with arsenic or phosphorus, negatively charged clusters of impurity atoms are formed that cause additional substantial changes in the diffusion process because of the change in the concentration of charge carriers and, correspondingly, in the internal electric field in the doped region.

The purpose of this work was to obtain and investigate the equation of diffusion of impurity atoms in a silicon plate. In explicit form this equation defines the influence of charged clusters on the process of impurity transfer.

Diffusion Equation of Impurity Atoms. We consider the most common case of diffusion of impurity atoms in a silicon plate by means of formation, migration, and disintegration of the "impurity atom–intrinsic point defect" pairs that are in a state of local thermodynamic equilibrium with impurity atoms in the substitution position and with nonequilibrium point defects. Let us assume that defects of one kind — vacancies or interstitial atoms of silicon — participate in the process of transfer of impurity atoms. The diffusion of impurity will then be described by the equation obtained in [4] which, in the one-dimensional case, can be presented in the following form:

$$\frac{\partial C^{\mathrm{t}}}{\partial t} = \frac{\partial}{\partial x}\left\{D(\chi)\left[\frac{\partial(\tilde{C}^{\mathrm{n}}C)}{\partial x} + \frac{\tilde{C}^{\mathrm{n}}C}{\chi}\frac{\partial \chi}{\partial x}\right]\right\}, \tag{1}$$

where

$$C^{\mathrm{t}} = C + C^{\mathrm{a,c}} . \tag{2}$$

It was shown in [2, 3] that in the case of charged clusters, the concentration of charge carriers χ reduced to n_i can be described by the expression

$$\chi = \frac{C + \dfrac{zz_{\mathrm{c}}}{m}C^{\mathrm{a,c}} - C^{\mathrm{b}} + \sqrt{\left(C + \dfrac{zz_{\mathrm{c}}}{m}C^{\mathrm{a,c}} - C^{\mathrm{b}}\right)^2 + 4n_i}}{2n_i}, \tag{3}$$

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where

$$C^{\mathrm{a,c}} = K\tilde{C}_{\mathrm{c}}\chi^{(m-z_{\mathrm{c}})}C^{m} \ , \tag{4}$$

$$\tilde{C}_{\mathrm{c}} = \frac{(\tilde{C}_{\mathrm{d1}})^{m_1}}{(\tilde{C}_{\mathrm{d2}})^{m_2}} \ , \quad \tilde{C}_{\mathrm{d1}} = \frac{C^{\mathrm{n}}_{\mathrm{d1}}}{C^{\mathrm{n}}_{\mathrm{d1eq}}} \ , \quad \tilde{C}_{\mathrm{d2}} = \frac{C^{\mathrm{n}}_{\mathrm{d2}}}{C^{\mathrm{n}}_{\mathrm{d2eq}}} \ . \tag{5}$$

The obtained diffusion equation, describing the evolution of the distribution of impurity atom concentration C, involves the derivative $\partial\chi/\partial x$. This means that this second-order partial differential equation is also nonlinear. To carry out an analysis of the characteristic features of the diffusion process, it is meaningful to transform this equation into a linear differential equation with nonlinear coefficients. For this purpose, we will calculate the derivative $\partial\chi/\partial x$. We introduce the notation $l_{\chi} = m - z_{\mathrm{c}}$ and rewrite expressions (4) and (3) in the following form:

$$C^{\mathrm{a,c}} = A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}C^{m} \ , \tag{6}$$

$$\chi = \frac{C + A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}C^{m} - C^{\mathrm{b}} + \sqrt{\left(C + A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}C^{m} - C^{\mathrm{b}}\right)^{2} + 4n_i^{2}}}{2n_i} , \tag{7}$$

where

$$A_{\mathrm{c}} = \frac{zz_{\mathrm{c}}}{m} K \ . \tag{8}$$

The partial derivative $\partial\chi/\partial x$ can be presented in the form

$$\frac{\partial\chi}{\partial x} = \frac{\partial\chi}{\partial C}\frac{\partial C}{\partial x} + \frac{\partial\chi}{\partial\tilde{C}_{\mathrm{c}}}\frac{\partial\tilde{C}_{\mathrm{c}}}{\partial x} + \frac{\partial\chi}{\partial C^{\mathrm{b}}}\frac{\partial C^{\mathrm{b}}}{\partial x} \ . \tag{9}$$

Let us calculate the derivatives $\partial\chi/\partial x$, $\partial\chi/\partial C^{\mathrm{b}}$, and $\partial\chi/\partial\tilde{C}_{\mathrm{c}}$:

$$\frac{\partial\chi}{\partial C} = \chi \frac{1 + A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}mC^{m-1}}{\sqrt{\left(C + A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}C^{m} - C^{\mathrm{b}}\right)^{2} + 4n_i^{2}} - A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}C^{m}} \ , \tag{10}$$

$$\frac{\partial\chi}{\partial\tilde{C}_{\mathrm{c}}} = \chi \frac{A_{\mathrm{c}}\chi^{l_{\chi}}C^{m}}{\sqrt{\left(C + A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}C^{m} - C^{\mathrm{b}}\right)^{2} + 4n_i^{2}} - A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}l_{\chi}\chi^{l_{\chi}}C^{m}} \ , \tag{11}$$

$$\frac{\partial\chi}{\partial C^{\mathrm{b}}} = -\chi \frac{1}{\sqrt{\left(C + A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}C^{m} - C^{\mathrm{b}}\right)^{2} + 4n_i^{2}} - A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}l_{\chi}\chi^{l_{\chi}}C^{m}} \ . \tag{12}$$

In the final outcome we obtain

$$\frac{1}{\chi}\frac{\partial\chi}{\partial x} = h^{\mathrm{b}}\frac{\partial C}{\partial x} + h^{\mathrm{c}}\frac{\partial C}{\partial x} - h^{\mathrm{c}}\frac{\partial C^{\mathrm{b}}}{\partial x} \ , \tag{13}$$

where

$$h^{\mathrm{b}}\left(C, \chi, \tilde{C}_{\mathrm{c}}, C^{\mathrm{b}}\right) = \frac{1 + A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}mC^{m-1}}{\sqrt{\left(C + A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}C^{m} - C^{\mathrm{b}}\right)^{2} + 4n_i^{2}} - A_{\mathrm{c}}\tilde{C}_{\mathrm{c}}\chi^{l_{\chi}}C^{m}} \ , \tag{14}$$