Simulation of point defect diffusion in structures with local elastic stresses

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The stress-mediated diffusion of nonequilibrium point defects from the surface to the bulk of the semiconductor is investigated by computer simulation. It is supposed that point defects are generated in the surface region by ion implantation and during diffusion pass over the local region of elastic stresses because the average defect migration length is greater than the thickness and depth of the strained layer. Within the strained layer point defect segregation or heavily defect depletion occur if defect drift under stresses is directed respectively in or out of the layer. On the other hand, the calculations show that, in contrast to the case of local defect sink, the local region of elastic stresses practically does not change the distribution of defects beyond this region if there is no generation/absorption of point defects within the strained layer.

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I. INTRODUCTION

In recent years decreasing dimensions of the integrated components especially with various multilayered structures such as Si/SiGe and the use of different nano-particles embedded in the crystalline matrix have been the main trends of advanced device technologies. Much attention is given to studying the defect kinetics and stress evolution during semiconductor processing because defect and stress engineering can significantly improve the device performance. For example, many efforts are directed to a study of the stress-mediated diffusion of impurity atoms and point defects including the influence of elastic stresses on the drift of point defects near the surface or at the interfaces and near different inhomogeneities of semiconductor crystals. Also, many studies are associated with changes in the defect subsystem of ion-implanted layers as these changes are responsible for the transient enhanced diffusion of dopant atoms. For example, to explain the experimental data, it is assumed that elastic stresses arising in the region of the SiGe layer buried in silicon and compressively strained after growth cause the drift of vacancies to this layer. Thus, accumulation of the vacancies within the layer and their transformation into nanovoids occur. In the transient enhanced diffusion of dopant atoms in hyperfine boron-doped layers created by the molecular-beam epitaxy is investigated experimentally. It is assumed that the formation of the clusters of boron atoms with silicon self-interstitials occurs in these doped regions during thermal treatment. This process and a number of similar thermal treatments are characterized by the local absorption of self-interstitials. Thus, investigations concerning the influence of the local strained regions and local sinks on the diffusion of nonequilibrium point defects are of great importance for the next-generation fabrication processes.

II. MODEL OF STRESS-MEDIATED DIFFUSION OF POINT DEFECTS

To calculate distributions of the nonequilibrium point defect concentration in the field of elastic stresses, the stationary diffusion equation established in Ref. can be used. In the form convenient for numerical solution this equation can be written as

$$\frac{d}{dx} \left[ C^C(\chi) \frac{d(a^d \tilde{C})}{dx} \right] - d(v_x \tilde{C})_x - \frac{k^C(\chi) k^{Sp}(x) a^d \tilde{C}}{l^2_i} + \frac{1 + \tilde{g}^R}{l^2_i} = 0,$$

where

$$\tilde{C} = \frac{C^\chi}{C^i}, \quad d^C(\chi) = \frac{d(\chi)}{d_i},$$

$$\chi = \frac{C - C_B + \sqrt{(C - C_B)^2 + 4n_i^2}}{2n_i},$$

$$v_x = -d^C(\chi) \frac{a^d}{k_B T} \frac{dU^d}{dx},$$

$$\tilde{g}^R = \frac{g^R}{g_i}.$$
dopant atoms forming a doped region; $C_B$ is the total concentration of dopant atoms responsible for opposite-type conductivity; $n_i$ is the intrinsic carrier concentration; $k^C(\chi)$ is the normalized to $k_1$ concentration dependence of the effective absorption coefficient for point defects; $k^{\delta p}(x)$ is the spatial distribution of the absorption coefficient; $k_1$ and $\tau_i = k_1^{-1}$ are the values of absorption coefficient and average lifetime for point defects in intrinsic semiconductor, respectively; $l_i = \sqrt{d_i \tau_i}$ is the average migration length of point defects in intrinsic semiconductor; $v_x$ is the $x$-coordinate projection of the effective drift velocity of point defects due to elastic stresses; $U^d$ is the potential energy of these defects in the field of elastic stresses; $\gamma^R$ is the rate of the nonequilibrium point defect generation per unit volume due to the external radiation or dissolution of extended defects; $g_i$ is the rate of thermally equilibrium generation of point defect in intrinsic semiconductor. The function $a^d = h^r/h_1^r$ takes into account that the real constants $h^r$ for the transition between the charge states of point defects deviate from their equilibrium values $h_1^r$ due to heavy doping effects and elastic stresses.

Eq. (1) differs from the defect diffusion equation used in Ref. 19,20 because the drift of mobile species in the field of elastic stresses is included. On the other hand, from Eq. (1) the distributions of nonequilibrium point defects can be derived, instead of computing the equilibrium defect distributions by means of expressions used in Ref. 19,20.

Eq. (1) is also convenient for numerical solutions due to the following characteristic features: (i) This equation describes the diffusion-reaction-drift of nonequilibrium point defects with different charge states as a whole, although only the normalized concentration of the neutral defects $\tilde{C}$ must be obtained to solve the equation. (ii) The obtained equation takes into account the drift of all charged species due to the built-in electric field. At the same time, there is no explicit term describing this drift. (iii) Despite the fact that the effective coefficients of Eq. (1) represent nonlinear functions of $\chi$, these functions are smooth and monotone. 21

It is also assumed that the mobility of point defects is significantly greater than the impurity atom mobility, and there is no change in the processing conditions or the changes are sufficiently slow. In this case the time derivative of the defect concentration is close to zero and distributions of point defects are quasi-stationary with respect to the distributions of dopant atoms, clusters, extended defects, and also with respect to changes in the processing conditions.

III. NUMERICAL SOLUTION

The finite-difference method is used to find a numerical solution for Eq. (1) in the one-dimensional (1D) domain $[0, x_B]$. Following Ref. 21, the first term in the left-hand side of Eq. (1) is approximated by a symmetric difference operator of the second order accuracy on the space variable $x$. At the same time, the second term is approximated with the first order accuracy by the asymmetric forward/backward-difference operator depending on the drift direction. On the other hand, if the defect flux due to elastic stresses is comparable to or below the defect flux due to the concentration gradient, the second term is also approximated by a symmetric difference operator of the second order accuracy. Comparison with exact analytical solutions for the particular cases of point defect diffusion and calculations on the meshes with different step sizes were carried out to verify the approximate numerical solution.

For example, in Fig. 1 the numerical solution for Eq. (1) in case of the constant diffusivity and constant coefficient of defect absorption is presented. For comparison with the analytical solution Gaussian distribution

$$\tilde{g}^R(x) = \tilde{g}_m \exp \left[ -\frac{(x - R_{pd})^2}{2\Delta R_{pd}^2} \right]$$

is used to describe the generation rate profile. Here $\tilde{g}_m$ is a maximum generation rate of point defect during ion implantation normalized to the thermal generation rate $g_i$; $R_{pd}$ and $\Delta R_{pd}$ are the position of a maximum of defect generation distribution and dispersion of this distribution, respectively. It is supposed that the defect generation occurs due to implantation of hydrogen ions at energy 20 keV ($R_{pd} = 0.198$ $\mu$m and $\Delta R_{pd} = 0.0802$ $\mu$m are taken from Ref. 24). Numerical computations are carried out on the simulation domain $[0, x_B]$, where $x_B$ and mesh point number $i_B$ are equal to 4.0 $\mu$m and 81, respectively. To obtain a numerical solution, the Dirichlet boundary conditions are imposed on $\tilde{C}$

$$\tilde{C}(0) = 1, \quad \tilde{C}(x_B) = 1.$$
The function \( \tilde{C}_{th}(x) = 1 \) is added to the analytical solution to satisfy boundary conditions and take into account the thermal generation of point defects. As can be seen from Fig. 1, the distribution of nonequilibrium point defects obtained by numerical computations agrees with the analytical solution proposed in Ref. 23.

IV. SIMULATION OF POINT DEFECT DIFFUSION

In Fig. 2, the calculated distribution of nonequilibrium point defects in the structure with the local stress field providing the drift of defects into the strained region is demonstrated. For comparison, the solution of diffusion equation in case of zero stresses is also shown by the dotted line.

![Fig. 2: Calculated distribution of the concentration of neutral point defects passing over the region of local stresses (drift velocity directed into the strained layer). A solution for the same diffusion equation in case of zero stresses is given for comparison.](image)

![Fig. 3: Spatial distribution of the normalized drift velocity of point defects used in calculations shown in Fig. 2.](image)

To meet the experiments with the transient enhanced diffusion, in all the calculations presented here it is assumed that the generation of nonequilibrium point defects occurs due to silicon ion implantation at an energy of 60 keV (\( R_p = 0.081 \) µm and \( \Delta R_p = 0.033 \) µm are also from Ref. 23), i.e. the generation occurs near the surface of the semiconductor. Here \( R_p \) and \( \Delta R_p \) are the average projective range of silicon ions and straggling of the projective range, respectively. To describe the defect diffusion, the average migration length of point defects is chosen equal to 0.7 µm to be greater than the thickness of the strained layer. The reflecting condition for point defects on the surface and Dirichlet condition in the bulk of semiconductor are used in all cases under consideration.

The distribution of the normalized drift velocity of point defects in the field of elastic stresses for the case of defect segregation within the local strained region (see Fig. 2) is given in Fig. 3. As can be seen from Fig. 3, the local field of elastic stresses takes place between the defect generation region and the bulk of the semiconductor.

Fig. 4 presents the calculated distribution of nonequilibrium point defects in the structure with the local region of stresses preventing the defect diffusion into the strained layer. The distribution of the normalized drift velocity of point defects in the field of elastic stresses used for this calculation is shown in Fig. 5. As can be seen from Fig. 5, it is supposed that the local stress field also occupies a position between the defect generation region and the bulk.

![Fig. 4: Calculated distribution of the concentration of neutral point defects passing over the region of local stresses (drift velocity directed out of the strained layer). A solution for the same diffusion equation in case of zero stresses is given for comparison.](image)

![Fig. 5: Calculated distribution of the concentration of neutral point defects passing over the region of local stresses (drift velocity directed out of the strained layer). A solution for the same diffusion equation in case of zero stresses is given for comparison.](image)

As seen from Figs. 2 and 4, the presence of the local stresses results either in enrichment or depletion of the stress region by point defects. On the other hand, the distributions of nonequilibrium defects beyond the region of the local stresses are practically unchanged, regardless of the stress region by point defects. On the other hand, the distributions of nonequilibrium defects beyond the region of the local stresses are practically unchanged, regardless of the stress region by point defects migrating in the bulk of the semiconductor.

A qualitatively different situation takes place in the
FIG. 5: Spatial distribution of the normalized drift velocity of point defects used in calculations shown in Fig. 4.

case of strong local sinks of point defects, for example, in the case of the silicon structure with an epitaxially grown Si$_{1-x}$C$_x$ layer. This can be seen in Fig. 6 showing the point defect concentration profile calculated for the local sink position at the same place as the position of local stresses in the previous calculations. Fig. 7 demonstrates the spatial distribution for the effective absorption coefficient of point defects used in the last calculation.

FIG. 6: Calculated distribution of the concentration of neutral point defects passing over the region of local sink. For comparison a solution of the diffusion equation for the thermally equilibrium uniform absorption of point defects is also presented.

A significant decrease in defect concentrations in the regions before and after the sink is easily predictable and agrees with the experimental data obtained in Ref. 20.

FIG. 7: Spatial distribution of the effective coefficient of point defect absorption used in calculations presented on Fig. 6.

FIG. 5: Spatial distribution of the normalized drift velocity of point defects used in calculations shown in Fig. 4.

V. CONCLUSIONS

The influence of local elastic stresses on the formation of point defect distributions during diffusion of nonequilibrium defects from the surface into the bulk of the semiconductor has been investigated by computer simulation. Such local regions of stresses can be formed in the multilayered heterostructures or semiconductor structures with heavily doped layers. Thus, point defects diffusing into the bulk must pass over the region of stresses if the average defect migration length is greater than the thickness of the strained layer. Within the strained layer, the point defect segregation or heavy defect depletion occur if the defect drift under stresses is directed respectively in or out of the layer. The numerical calculations show that, in contrast to the case of local defect sink, the local region of elastic stresses practically does not change the distribution of defects beyond this region provided that there is no generation/absorption of point defects within the strained layers.

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