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ANALYTICAL SOLUTION OF EQUATIONS SET DESCRIBING DIFFUSION OF POINT DEFECTS IN THE 2-LAYER SEMICONDUCTOR STRUCTURE

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Abstract. The boundary-value problem on impurity and point defect diffusion in the 2-layer semiconductor structure was formulated and analyzed. The analytical solution of the set of equations describing diffusion of intrinsic point defects was obtained for the case of the constant coefficients of these equations. Calculation of the typical distribution of point defects in the 2-layer structure was carried out.

Keywords: silicon, SiGe, impurity, defect, diffusion equation, analytical solution.

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Introduction

At present, different layered structures such as «silicon on insulator» or SOI [1], $Si/Si_{1-x}Ge_x$ [2] and others are widely used with the purpose to improve the electric parameters of semiconductor devices and integrated microcircuits. It is worth noting that although Si and Ge relate to the elements of the IVth group of the Mendeleev's law, the properties of the band gap can vary significantly in the layers of SiGe [3]. The goal of the research presented below is investigation of the characteristic features of diffusion of impurity atoms and intrinsic point defects in such layered structures.

The boundary-value problem on impurity and defect diffusion

Let consider for the sake of simplicity a 2-layer system in the one-dimensional (1D) case. In general, the boundary conditions on the surface and in the bulk of a semiconductor can be presented in the following form:

$$w_1^S j_x\Big|_{x=0} + w_2^S C(0,t) = w_3^S,\ w_1^B j_x\Big|_{x=x_B} + w_2^B C(x_B,t) = w_3^B, \quad (1)$$

$$w_1^{Sd} j_x^d\Big|_{x=0} + w_2^{Sd} C^d(0,t) = w_3^{Sd},\ w_1^{Bd} j_x^d\Big|_{x=x_B} + w_2^{Bd} C^d(x_B,t) = w_3^{Bd}. \quad (2)$$

Here C and j_x are the impurity concentration and the x-coordinate projection of the impurity flux, respectively; x_B is the position of the right boundary of the second layer; C_B is the concentration of impurity atoms on this boundary; C^d and j_x^d are the concentrations of point defects (vacancies or intrinsic interstitial atoms) and the x-coordinate projection of the flux of this species, respectively; w_1, w_2, w_3 are the constant coefficients specifying the Dirichlet, reflecting or the Robin boundary conditions for impurity atoms and point defects.

The condition of the flux continuity of the impurity atoms on the interface between the layers

located at $x = x_{12}$ is added to equations (1) and (2):

$$j_x\big|_{x=x_{12}-0} = j_x\big|_{x=x_{12}+0}. \quad (3)$$

It is supposed for simplicity that there is no generation or absorption of intrinsic point defects on the interface and the condition of the flux continuity of the intrinsic point defects can be used:

$$j_x^d\big|_{x=x_{12}-0} = j_x^d\big|_{x=x_{12}+0}. \quad (4)$$

It is well known that the electrochemical potentials for impurity atoms and point defects are the continuous functions across the interface [4]:

$$\left(\mu_1 + z_1 e\varphi_1\right)\big|_{x=x_{12}-0} = \left(\mu_2 + z_2 e\varphi_2\right)\big|_{x=x_{12}+0}, \quad (5)$$

$$\left(\mu_1^d + z_1^d e\varphi_1\right)\big|_{x=x_{12}-0} = \left(\mu_2^d + z_2^d e\varphi_2\right)\big|_{x=x_{12}+0}, \quad (6)$$

where μ and μ^d are the chemical potentials of impurity atoms and intrinsic point defects, respectively; z and z^d are respectively the charge of substitutionally dissolved impurity atoms and the charge of the point defect, expressed in terms of the elementary charge; φ is the potential of the built-in electric field. The subscripts 1 and 2 describe the values of physical magnitudes under consideration in the first and in the second layers, respectively. It is worth noting that this statement does not relate to the parameters w.

In the case of ideal solubility, the chemical potential of the species is defined by the expressions [4]

$$\mu = \mu_0(T) + k_B T \ln C, \ \mu^d = \mu_0^d(T) + k_B T \ln C^d. \quad (7)$$

It is clear from expressions (7), that the continuity of the electrochemical potential can cause the discontinuity in the values of the concentration of atomic species on the right and left hands of the interface. Therefore, in modeling impurity diffusion in the silicon dioxide / silicon (SiO_2/Si) system condition (5) is usually replaced by the condition

$$\left.\frac{C_1}{C_2}\right|_{x=x_{12}} = k_S, \quad (8)$$

where k_S is the empirical coefficient describing the segregation of impurity atoms on the SiO_2/Si interface [5].

We can use a similar technique to model diffusion of intrinsic point defects. With this purpose, condition (6) is replaced by the ratio

$$\left.\frac{C_1^d}{C_2^d}\right|_{x=x_{12}} = k_S^d, \quad (9)$$

where k_S^d is the empirical coefficient describing the segregation of point defects on the interface located at $x = x_{12}$.

Unlike the impurity atoms, the intrinsic point defects can be in different charge states. Therefore, to describe their diffusion it is necessary to use a set of diffusion equations written for the each charge state. However, using the mass action law, one can reduce this set to one generalized equation of the diffusion of point defects in the neutral charge state [6]. It is very convenient for a qualitative analysis and quantitative calculations of point defect distributions because the built-in electric field does not exert a direct influence on the diffusion of neutral particles. Moreover, the concentration of impurity atoms in the position of replacement is close to, or less than concentration of intrinsic charge carriers at a treatment temperature (n_i). Then, the coefficients of the generalized diffusion equation are constants. The latter condition is also valid in the case of the significant fraction of neutral point defects participating in diffusion. It is necessary to note that the description of diffusion of point defects by means of the equation with constant coefficients

is a very good approximation due to the wide uncertainty of the parameters describing the transport processes of these species [7]. Taking into account the analysis given above and the high mobility of vacancies and silicon self-interstitials in comparison with the mobility of impurity atoms, one can describe the diffusion of point defects in the 2-layer structure under consideration by two stationary diffusion equations involving constant coefficients and having the form proposed in [6]:

$$\frac{d^2 \tilde{C}_1^{\times}}{d x^2} - \frac{\tilde{C}_1^{\times}}{l_{1i}^2} + \frac{\tilde{g}_1}{l_{1i}^2} = 0, \tag{10}$$

$$\frac{d^2 \tilde{C}_2^{\times}}{d x^2} - \frac{\tilde{C}_2^{\times}}{l_{2i}^2} + \frac{\tilde{g}_2}{l_{2i}^2} = 0, \tag{11}$$

where $\tilde{C}^{\times}$ is the concentration of point defects under consideration in the neutral charge state $C^{\times}$ normalized to the thermally equilibrium value $C_{eq}^{\times}$; $l_i = \sqrt{d_i \tau_i}$ is the average migration length of these defects; d_i and τ_i are the diffusivity and average life time of the point defects in an intrinsic semiconductor, respectively; $\tilde{g} = 1 + G_R / G_{eq}$, where G_R and G_{eq} are the rate of the generation of point defects per unit volume due to external irradiation and the rate of the thermal generation of these defects, respectively.

Analytical solution

Let obtain the analytical solution of the set of equations (10) and (11) for the Dirichlet boundary conditions:

$$\tilde{C}_1^{\times}(0) = \tilde{C}_S^{\times},\ \tilde{C}_1^{\times}(x_{12}) = \tilde{C}_{1L}^{\times},\ \frac{\tilde{C}_{1L}^{\times}}{\tilde{C}_{2R}^{\times}} = k_S^d,\ \tilde{C}_2^{\times}(x_{12}) = \tilde{C}_{2R}^{\times},\ \tilde{C}_2^{\times}(x_B) = \tilde{C}_B^{\times}, \tag{12}$$

where $\tilde{C}_S^{\times}$ and $\tilde{C}_B^{\times}$ are the normalized concentration of the neutral point defects on the surface of a semiconductor and on the right boundary of the second layer.

This solution has the form:

$$\tilde{C}_1^{\times}(x) = \tilde{g}_1 + C_{11} \exp\left(-\frac{x}{l_{1i}}\right) + C_{12} \exp\left(\frac{x}{l_{1i}}\right), \tag{13}$$

$$\tilde{C}_2^{\times}(x) = \tilde{g}_2 + C_{21} \exp\left(-\frac{x}{l_{2i}}\right) + C_{22} \exp\left(\frac{x}{l_{2i}}\right), \tag{14}$$

where

$$C_{11} = \frac{\exp\left(\frac{x_{12}}{l_{1i}}\right)\left[k_S^d \tilde{C}_{2R}^{\times} - \tilde{g}_1 + \left(\tilde{g}_1 - \tilde{C}_S^{\times}\right)\exp\left(\frac{x_{12}}{l_{1i}}\right)\right]}{1 - \exp\left(\frac{2x_{12}}{l_{1i}}\right)}, \tag{15}$$

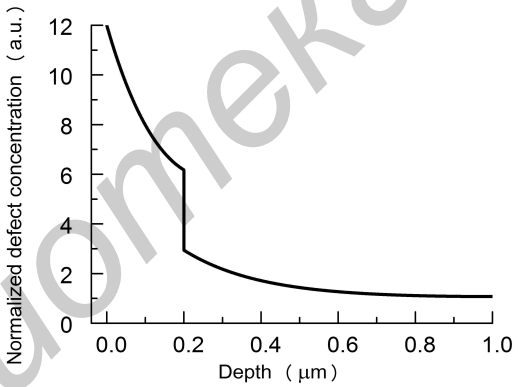
$$C_{12} = \frac{\tilde{C}_S^{\times} - \tilde{g}_1 + \left(\tilde{g}_1 - k_S^d \tilde{C}_{2R}^{\times}\right)\exp\left(\frac{x_{12}}{l_{1i}}\right)}{1 - \exp\left(\frac{2x_{12}}{l_{1i}}\right)}, \tag{16}$$

$$C_{21} = \frac{\left(\tilde{C}_{2R}^{\times} - \tilde{g}_2\right)\exp\left(\frac{x_{12} + 2x_B}{l_{2i}}\right) + \left(\tilde{g}_2 - \tilde{C}_B^{\times}\right)\exp\left(\frac{2x_{12} + x_B}{l_{2i}}\right)}{\exp\left(\frac{2x_B}{l_{2i}}\right) - \exp\left(\frac{2x_{12}}{l_{2i}}\right)}, \tag{17}$$

$$C_{22} = -\frac{\left(\tilde{C}_{2R}^{\times} - \tilde{g}_2\right)\exp\left(\frac{x_{12}}{l_{2i}}\right) + \left(\tilde{g}_2 - \tilde{C}_B^{\times}\right)\exp\left(\frac{x_B}{l_{2i}}\right)}{\exp\left(\frac{2x_B}{l_{2i}}\right) - \exp\left(\frac{2x_{12}}{l_{2i}}\right)}, \tag{18}$$

$$\begin{aligned}
\tilde{C}_{2R} = &\left\{2d_{2i}\, l_{1i}\tilde{C}_B \exp\left(\frac{2x_{12}+x_B}{l_{2i}}\right)\left[1-\exp\left(\frac{2x_{12}}{l_{1i}}\right)\right] + \left[\exp\left(\frac{x_{12}}{l_{2i}}\right) - \exp\left(\frac{x_B}{l_{2i}}\right)\right]\right. \\
&\times\left\{d_{2i}\, l_{1i}\tilde{g}_2\left[1-\exp\left(\frac{2x_{12}}{l_{1i}}\right)\right]\left[\exp\left(\frac{x_{12}}{l_{2i}}\right) - \exp\left(\frac{x_B}{l_{2i}}\right)\right] + d_{1i}\, l_{2i}\frac{C_{eq1}^{\times}}{C_{eq2}^{\times}}\left[\exp\left(\frac{x_{12}}{l_{2i}}\right) + \exp\left(\frac{x_B}{l_{2i}}\right)\right]\right. \\
&\times\left.\left\{2\tilde{C}_S^{\times}\exp\left(\frac{x_{12}}{l_{1i}}\right) + \tilde{g}_1\left[1-\exp\left(\frac{x_{12}}{l_{1i}}\right)\right]^2\right\}\right\}\left\{d_{2i}\, l_{1i}\left[1-\exp\left(\frac{2x_{12}}{l_{1i}}\right)\right]\left[\exp\left(\frac{2x_{12}}{l_{2i}}\right) + \exp\left(\frac{2x_B}{l_{2i}}\right)\right]\right. \\
&\left.+d_{1i}k_S^d\, l_{2i}\frac{C_{eq1}^{\times}}{C_{eq2}^{\times}}\left[1+\exp\left(\frac{2x_{12}}{l_{1i}}\right)\right]\left[\exp\left(\frac{2x_{12}}{l_{2i}}\right) - \exp\left(\frac{2x_B}{l_{2i}}\right)\right]\right\}^{-1}.
\end{aligned} \tag{19}$$

Figure presents the typical results of calculation of the distribution of point defects in the 2-layer structure, carried out with the help of the obtained analytical solution. It is supposed that the point defects are generated on the surface of a semiconductor and that the coefficient describing the segregation of point defects is higher than 1 ($k_S^d = 2.1$). The following values of the parameters of diffusion of point defects have been used: $\tilde{C}_S^{\times} = 12$ a.u.; $\tilde{C}_B^{\times} = 1$ a.u.; $x_{12} = 0.2$ μm; $l_{1i} = 0.18$ μm; $l_{2i} = 0.2$ μm; $d_{1i} = d_{2i}$; $\tilde{g}_1 = \tilde{g}_2 = 1.0$ a.u.



Calculated distribution of the concentration of nonequilibrium neutral point defects in the 2-layer structure. The segregation coefficient for point defects is equal to 2.1

It can be seen from figure that the discontinuity of the concentration of point defects occurs on the interface at $k_S^d \neq 1$. This discontinuity can significantly influence the diffusion of impurity atoms in the vicinity of the interface. It is necessary to note that the analytical solution obtained can be used to check the numerical solutions describing diffusion of point defects in the 2-layer structures.

Conclusions

The boundary-value problem on impurity and point defect diffusion in the 2-layer semiconductor structure has been formulated and analyzed. The analytical solution of the set of equations describing diffusion of intrinsic point defects in this structure was obtained, and calculation of the typical distribution of nonequilibrium point defects was carried out. The analytical solution obtained can be used for checking the numerical solutions in the course of development of the numerical methods and codes for modeling the transports processes in layered structures.

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