Vol. **110** (2006) *ACTA PHYSICA POLONICA A* No. 4

# Fast Diffusion of Metastable Vacancies in Surface of Excited Si Crystals

A.J. Janavičius[a,*] and S. Turskienė[b]

[a]Faculty of Natural Sciences, Šiauliai University
Višinskio 25, Šiauliai, 76351, Lithuania

[b]Faculty of Mathematics and Informatics, Šiauliai University
Višinskio 19, Šiauliai, 76351, Lithuania

*(Received June 19, 2006)*

We considered the practically interesting, very fast nonlinear diffusion of metastable vacancies in the surface of Si crystal, excited by soft X-rays. Here we used experimentally defined diffusion coefficients of singly and doubly negatively charged very fast vacancies generated by soft X-rays. These high concentration (about $10^{13}$ cm$^{-3}$) metastable vacancies at room temperature can diffuse and exist in the crystal for a very long time (about 24 hours for not so fast neutral vacancies) changing electrical conductivity, the Hall mobility of carriers and generating some resonance phenomena in the lattice of Si crystal. We measured superdiffusivity of negatively charged vacancies, generated by the Auger effect in the regions of the sample, where X-rays did not acted. In the paper we modified the formerly obtained analytical solution of nonlinear diffusion equation for calculation of distribution of vacancies in two-dimensional surface.

PACS numbers: 66.30.–h, 66.30.Hs, 78.70.Ck

## 1. Introduction

We considered the superdiffusivity [1] of metastable vacancies [2] in the surface of crystal silicon irradiated by soft X-rays. Excited vacancies can be produced by moving of the atoms from the lattice sites into neighboring metastables states with 1 eV energies or to interstitial states with energies 0.8 eV [3] as a result of the Coulomb interaction after the ejection of the Auger electrons [3]. These atoms can penetrate into metastable states through barrier of height 1.5 eV [3]. For displacement into interstitial state they must penetrate through additional

*corresponding author

barrier 0.5 eV [3]. The irradiated vacancies superdiffusion is a result of the interaction between electrons transitions and the local lattice vibrations [4]. The local heating of atoms surrounding the excited vacancies can increase local temperature till 1300 K [2]. The obtained singly and doubly charged excited vacancies have diffusion coefficients [5, 6] $10^4$ times larger than vacancies obtained by thermal heating [7].

A very long duration of excited negative vacancies [5] (about 9 hours) and their superdiffusion at room temperature [2, 5, 6] created conditions for opening the superdiffusivity of impurities in excited Si crystal [7] and possibility of production of new microprocessors and solar cells. Mathematical investigation of excited vacancies diffusion [8] in surface of Si crystal can be useful for interpretation of experiments and modeling of new devices.

## 2. Analytical solution of the nonlinear diffusion equation

From the theory of Brownian motion it follows that mean displacement of chaotically moving particles is proportional to the square root of the time [9]. For diffusion in solids, where distance and time of elementary jumps are definite, diffusion velocity and the maximal penetration depths must be finite. Describing these physical conditions, the following nonlinear diffusion equation was proposed in our paper [10]:

$$j(x,t) = -D_n n(x,t)\frac{\mathrm{d}}{\mathrm{d}x}n(x,t), \quad \frac{\mathrm{d}}{\mathrm{d}t}n(x,t) = D_n\frac{\mathrm{d}}{\mathrm{d}x}\left[n(x,t)\frac{\mathrm{d}}{\mathrm{d}x}n(x,t)\right], \tag{1}$$

with the diffusion coefficient directly proportional to the concentration of impurities $n(x,t)$:

$$D(n) = D_n n(x,t). \tag{2}$$

In the paper [11] it was shown that

$$D_n = \frac{1}{N_\mathrm{S}}D_\mathrm{L}, \tag{3}$$

where $N_\mathrm{S}$ is impurities concentration at the source and $D_\mathrm{L}$ diffusion coefficient for linear diffusion equation.

Using above presented equation we can write the nonlinear diffusion equation in two-dimensional case

$$\frac{\mathrm{d}}{\mathrm{d}t}n(x,y,t) = \frac{\mathrm{d}}{\mathrm{d}x}\left[D_1(n)\frac{\mathrm{d}}{\mathrm{d}x}n\right] + \frac{\mathrm{d}}{\mathrm{d}y}\left[D_2(n)\frac{\mathrm{d}}{\mathrm{d}y}n\right]. \tag{4}$$

This equation was solved for the point source of impurities in paper [12]. We presented the obtained solution for the boundary condition

$$n(0,0,t) = N_\mathrm{S} \tag{5}$$

in the following form:

$$n(x,y,t) = N_\mathrm{S}f(\xi_1,\xi_2), \quad f(\xi_1,\xi_2) = a\xi_1 + a\xi_2 + b\xi_1^2 + b\xi_2^2 + c\xi_1\xi_2,$$
$$a = -0.316, \quad b = -0.500, \quad c = 2.50. \tag{6}$$

Here $N_\mathrm{S}$ is the constant impurities concentration at the source.

In the expression (6) of solution (4) we used similarity variables

$$\xi_1 = \frac{|x|}{\sqrt{D_{1\mathrm{L}}t}} - \xi_{10}, \quad \xi_2 = \frac{|y|}{\sqrt{D_{2\mathrm{L}}t}} - \xi_{20},$$

$$\xi_{10} = \xi_{20} = \xi_0 = 0.632, \quad -\xi_0 \le \xi_1 \le 0, \quad -\xi_0 \le \xi_2 \le 0 \tag{7}$$

and boundary conditions

$$f(-\xi_{10}, -\xi_{20}) = 1, \tag{8}$$

$$f(0, -\xi_{20}) = 0, \quad f(-\xi_{10}, 0) = 0. \tag{9}$$

From the presented expressions we can obtain the maximal distance which can be attained by diffusing particles

$$R_\mathrm{M} = \sqrt{x^2 + y^2} = \xi_0\sqrt{D_{1\mathrm{L}}t + D_{2\mathrm{L}}t}, \quad \xi_0 = 0.632. \tag{10}$$

For circle source with radii $R$ of diffusing particles we changed the similarity variables in the following way:

$$\xi_{1R} = \frac{|x| - R}{\sqrt{D_{1\mathrm{L}}t}} - \xi_0, \quad \xi_{2R} = \frac{|y| - R}{\sqrt{D_{2\mathrm{L}}t}} - \xi_0. \tag{11}$$

Here the absolute values of coordinates $x$ and $y$ must satisfy the conditions

$$R \le |x| \le R + \xi_0\sqrt{D_{1\mathrm{L}}t}, \quad R \le |y| \le R + \xi_0\sqrt{D_{2\mathrm{L}}t}. \tag{12}$$

Then solution of nonlinear diffusion Eq. (4) for two-dimensional case, when impurities are introduced in the circle, can be expressed like in (5) only with new variables (11). It is the result of the fact that derivatives in Eq. (4) using variables (11) instead (7) stay the same and the new boundary conditions (8), (9) can be presented in the same way

$$f(-\xi_0, -\xi_0) = 1, \tag{13}$$

$$f(0, -\xi_0) = 0, \quad f(-\xi_0, 0) = 0. \tag{14}$$

We can rewrite these conditions for function $f(x, y, t)$ with the following coordinates:

$$f(|x| = R, y = 0, t) = 1, \quad f(x = 0, |y| = R, t) = 1,$$

$$f(|y| = R + \xi_0\sqrt{D_{1\mathrm{L}}t}, |x| = R) = 0,$$

$$f(|x| = R + \xi_0\sqrt{D_{1\mathrm{L}}t}, |y| = R) = 0. \tag{15}$$

These approximate boundary conditions can describe nonlinear diffusion in the plane for square (area $4R^2$) or circle with radii $R$ sources sufficiently well at the distances

$$\xi_0\sqrt{D_{1\mathrm{L}}t + D_{2\mathrm{L}}t} > R. \tag{16}$$

## 3. Calculations of diffusion of metastable vacancies at the surface of excited Si crystal

Vacancies are rapid diffusers [13] with activation energies of migration: 0.18 eV for $V^{2-}$, 0.45 eV for $V^0$, 0.32 eV for $V^{2+}$. Usually it is accepted that

$V^-$ and $V^+$ have intermediate meanings. During diffusion the vacancies and interstitial may recombine with vacancies and interact with impurities.

In the paper [5] $p$-Si boron doped sample (boron concentration $4 \times 10^{13}$ cm$^{-3}$, crystal size $3.33 \times 3.06 \times 3.09$ mm$^3$) was irradiated by X-ray tube (DRON-2, Russian device, copper anode voltage 11 kV and current 50 mA) at room temperature $T = 290$ K. The obtained dependence of conductivity increasing on the square root of the irradiation time, presented as two connected straight lines, were used for definition of diffusion coefficients and concentrations of irradiated negative vacancies. Sample was saturated by negative vacancies for a time $t = 3.2 \times 10^4$ s. Considering that most rapid diffuser is double charged negative vacancies [13], we can present diffusion coefficients and concentrations of irradiated vacancies in the following way:

$$D^{-2} = 3.05 \times 10^{-4}\ \mathrm{mm}^2/\mathrm{s}, \quad N_{\mathrm{S}}^{-2} = 0.539 \times 10^{10}\ \mathrm{mm}^{-3}, \tag{17}$$

$$D^{-} = 1.47 \times 10^{-4}\ \mathrm{mm}^2/\mathrm{s}, \quad N_{\mathrm{S}}^{-} = 0.286 \times 10^{10}\ \mathrm{mm}^{-3}. \tag{18}$$

In the paper [5] it was obtained that photons with maximum energies 11 keV can penetrate only to depth $d = 6.9 \times 10^{-2}$ mm and vacancies are generated only in this thin layer of surface. Using (6) and (11) for irradiated surface in the circle with radius $R = 0.5$ mm and above presented parameters we calculated the distributions of irradiated negative vacancies in Si crystal surface. Distributions of concentrations of singly and doubly charged negative vacancies, for irradiation time $t = 3.2 \times 10^4$ s of Si crystal, are presented in Fig. 1, Fig. 2, and Fig. 3, Fig. 4, consequently.

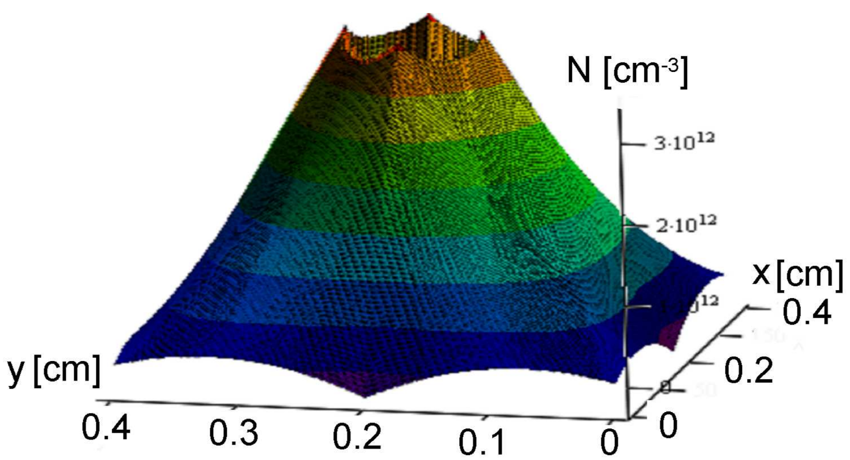


Fig. 1. Surface plot of distribution of concentrations of singly negatively charged vacancies for irradiated Si crystal in the circle with radius $R = 0.05$ cm. Maximal distance $R_{\mathrm{M}}$ from irradiation center, which can be achieved by diffusing vacancies, for irradiation time $t = 3.2 \times 10^4$ s is 0.20 cm.

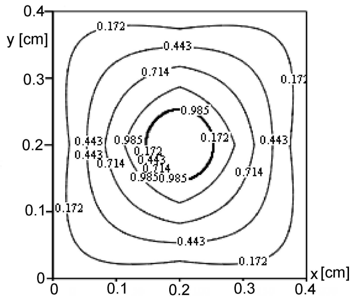


Fig. 2. Contour plot of distribution of relative concentrations of singly charged vacancies for irradiated Si crystal in the circle with radius $R = 0.05$ cm. Maximal distance $R_{\mathrm{M}}$, which can be achieved from irradiation center by diffusing vacancies, for irradiation time $t = 3.2 \times 10^4$ s is 0.20 cm.

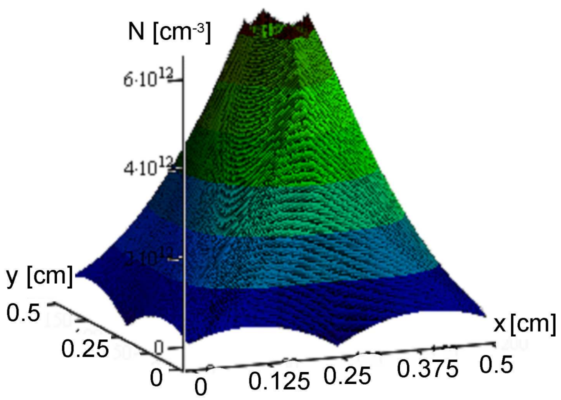


Fig. 3. Surface plot of distribution of concentrations of doubly charged vacancies for irradiated Si crystal in the circle with radius $R = 0.05$ cm. Maximal distance $R_{\mathrm{M}}$ from irradiation center, which can be achieved by diffusing vacancies, for irradiation time $t = 3.2 \times 10^4$ s is 0.25 cm.

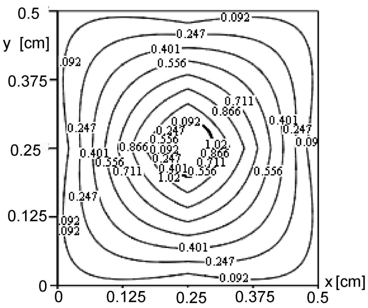


Fig. 4. Contour plot of distribution of relative concentrations of doubly charged vacancies for irradiated Si crystal in the circle with radius $R = 0.05$ cm. Maximal distance $R_{\mathrm{M}}$, which can be achieved from irradiation center by diffusing vacancies, for irradiation time $t = 3.2 \times 10^4$ s is 0.25 cm.

## 4. Conclusions

We presented approximate solutions which are sufficiently exact for evaluation of densities and amount of introduced charged metastable vacancies. These results can be used considering time dependence of the surface conductivity and definition of diffusion coefficients. Also the obtained solutions can be used for consideration of experiments when diffusion coefficient of vacancies depends on crystal orientation. Boundary conditions presented by first two formulae in (15) describe source and solution at great distances only approximately and we can see some distortions in the graphically presented solutions.

## References

[1] A.J. Janavičius, *Acta Phys. Pol. A* **93**, 505 (1998).

[2] A.J. Janavičius, J. Banys, R. Purlys, S. Balakauskas, *Lith. J. Phys.* **42**, 337 (2002).

[3] V.S. Vavilov, A.E. Kiv, O.R. Nijazova, *Mechanism of Producing and Migration of Defects in Semiconductors*, Science, Moscow 1981, p. 368.

[4] A.J. Janavičius, R. Purlys, Ž. Norgėla, *Acta Phys. Pol. A* **109**, 159 (2006).

[5] R. Purlys, A.J. Janavičius, A. Mekys, S. Balakauskas, J. Storasta, *Lith. J. Phys.* **41**, 376 (2001).

[6] A.J. Janavičius, Ž. Norgėla, R. Purlys, *Eur. Phys. J. Appl. Phys.* **29**, 127 (2005).

[7] A.J. Janavičius, *Science and Technique*, No. 12, *J. Lith. Acad. Eng. Union*, 2005, p. 19 (in Lithuanian).

[8] J.A. Van Vechten, *Phys. Rev. B* **10**, 1482 (1974).

[9] C. Kittel, *Elementary Statistical Physics*, Wiley, Inc., London, Chapman & Hall, Ltd., New York 1958, p. 278.

[10] A.J. Janavičius, V. Stukaitė, D.J. Zanevičius, *Electron Techn. Ser. 2: Semiconductor Dev.* **160**, 27 (1983) (in Russian).

[11] A.J. Janavičius, *Phys. Lett. A* **224**, 159 (1997).

[12] A.J. Janavičius, S. Turskienė, *Acta Phys. Pol. A* **108**, 979 (2005).

[13] J.L. Hastings, S.K. Estreicher, P.A. Fedders, *Phys. Rev. B* **56**, 10215 (1997).