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STOCHASTIC THEORY OF CHARGE DYNAMICS AND RECOMBINATION IN DEFECT CLUSTERS IN BULK SILICON

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Various types of defect clusters are generated in bulk Si-based high-energy particle detectors. They become either recombination centres or charge trapping centres. Populated trapping centres create internal fields which may affect the dynamics and recombination of remaining free charges. In the semiclassical regime, the charge dynamics can be described by the Boltzmann equation. In this paper, the stochastic description is presented as an alternative to a direct solution of the Boltzmann equation approach. It is demonstrated that the hole dynamics can be described in the overdamped regime in both light-hole and heavy-hole cases. Electrons have to be described by including ballistic components. The theory allows an efficient simulation of the electron and hole dynamics in the vicinity of a defect cluster and demonstrates that local trapping centres are the major components enabling fast charge recombinations. The dipolar type internal fields of permanently trapped charges only weakly influence the charge recombination kinetics.

Keywords: stochastic Boltzmann equation, silicon, recombination kinetics

1. Introduction

Silicon-based semiconductor detectors are at the core of high-energy (HE) particle detectors in, e.g. Large Hadron Collider – LHC at CERN [1]. Their principle of operation is essentially the same as in any type of photodetection: the incoming flux of particles generate photocurrent, which is being detected. The HE particles generate not only mobile charges (electrons and holes). High energies of incoming particles yield various types of lattice point defects, which shorten the device lifetime and the detectors degrade [2, 3]. The avalanche-like defect generation of vacancies and interstitial atoms has been proposed [4]. Such conditions then create a non-uniform distribution of lattice defects and various clustering becomes possible [4, 5]. Some defects become recombination centres and thus open an additional channel of recombination. Other types of defects become charge trapping sites. As the material is neutral, if some charges are trapped, remaining charges redistribute, thus creating internal electric fields. Locally the internal fields may drive remaining free charges and thus can affect various electronic properties, e.g. charge recombination kinetics.

Microscopic studies of point defects in the Si crystal reveal several types of interstitials and vacancies [5–7] with their unique electronic properties. Point defects can essentially trap electrons or holes, while some are recombination centres. A non-homogeneous distribution of point defects after HE particle illumination creates defect clusters and local internal fields that affect the dynamics of the remaining charges on long distances [8]. A strong correlation between the type of defect clustering and the type of irradiation has been established [9, 10]. It has been estimated that the largest amount of defects are the recombination centres, which can be assumed to be distributed uniformly in the vicinity of (and within) the defect cluster. In the simplified picture, the charged defects thus create the 'polarized' medium for free charges and it thus presumably becomes a significant factor, which drives the free charges that become captured by neutral recombination centres.

Experimentally determined recombination kinetics reveals charge recombination rates and

demonstrates that the charge recombination time is directly proportional to the overall doze of irradiation [8]. It is not clear whether this variation of charge lifetime is due to the increase of overall defect density in the bulk or due to internal electric fields in the cluster. This question is addressed by computer simulations of the electron and hole dynamics in the vicinity of the simplest possible defect cluster. Coherent as well as overdamped charge dynamics is considered. It is demonstrated that overdamped dynamics results in a poor description of charges. This assumption yields a shortening of the recombination kinetics. In the coherent regime, it is remarkable that light holes and heavy holes also make a difference. Most importantly, it is found that the trapping centres are the determining factor which controls the recombination rate irrespective of the internal fields.

2. Theory of charge distribution in a bulk crystal

Describing charge recombination requires following the electron and hole density in the volume under consideration. In the semiclassical approximation, in the vicinity of the conduction band minimum and valence band maximum, the electron and hole quasiparticles are quantum wavepackets, characterized by their effective masses, while the evolution of their mean coordinates obeys the classical equations of motion. The velocity of an electron, as a quasiparticle, is the group velocity, which is related to the average momentum by $\boldsymbol{\upsilon} = \boldsymbol{p}/m_{\mathrm{c}}^{*}$; we thus use υ as the dynamic variable. The conjugate variable is the position r. Considering the electron and hole, the cumulative 12-dimensional distribution function and its time evolution has to be considered:

$$\dot{\rho}(\boldsymbol{u}_{\mathrm{e}}, \boldsymbol{u}_{\mathrm{h}}, t) = \boldsymbol{D}\hat{\Delta}\rho(\boldsymbol{u}_{\mathrm{e}}, \boldsymbol{u}_{\mathrm{h}}, t)$$

$$-\hat{\nabla} \cdot (\rho(\boldsymbol{u}_{\mathrm{e}}, \boldsymbol{u}_{\mathrm{h}}, t)\, \boldsymbol{F}(\boldsymbol{u}_{\mathrm{e}}, \boldsymbol{u}_{\mathrm{h}}, t))$$

$$-S(\boldsymbol{u}_{\mathrm{e}}, \boldsymbol{u}_{\mathrm{h}}, t)\, \rho(\boldsymbol{u}_{\mathrm{e}}, \boldsymbol{u}_{\mathrm{h}}, t). \quad (1)$$

Here an overdot denotes the time derivative, and $\boldsymbol{u}^{T} = (\boldsymbol{\upsilon}, \boldsymbol{r})$ is a 6-dimensional vector containing a momentum and a coordinate. This is the traditional Fokker–Planck equation describing the complete dynamics [11], however, its terms are complicated.

The first term on the right describes spreading of the density in the 12-dimensional space with $\hat{\Delta}$ being the generalized Laplacian, hence $\boldsymbol{D}$ is the 12×12 matrix. In the most general form it describes the diffusion of both coordinate and momenta. However, as electrons cannot 'diffuse' into holes, $\boldsymbol{D}$ splits into blocks for electrons and holes. Additionally, the diffusion of momentum can also be ignored, and only the diagonal diffusion elements of electrons and holes have to be considered. Consequently we have only two terms

$$\boldsymbol{D}\hat{\Delta} = D_{\mathrm{e}}\Delta_{r\mathrm{e}} + D_{\mathrm{h}}\Delta_{r\mathrm{h}}, \quad (2)$$

where D_{e} and D_{h} are the electron and hole diffusion coefficients, $\Delta_{r\mathrm{e}} = \partial_{x_{\mathrm{e}}}^2 + \partial_{y_{\mathrm{e}}}^2 + \partial_{z_{\mathrm{e}}}^2$ is the Laplacian for electron coordinates, and $\Delta_{r\mathrm{h}} = \partial_{x_{\mathrm{h}}}^2 + \partial_{y_{\mathrm{h}}}^2 + \partial_{z_{\mathrm{h}}}^2$ is the corresponding operator for holes. We will also use the nabla operators $\nabla_{r\mathrm{e}} = x\partial_{x_{\mathrm{e}}} + y\partial_{y_{\mathrm{e}}} + z\partial_{z_{\mathrm{e}}}$, $\nabla_{r\mathrm{h}} = x\partial_{x_{\mathrm{h}}} + y\partial_{y_{\mathrm{h}}} + z\partial_{z_{\mathrm{h}}}$ and the corresponding operators with respect to the velocity $\nabla_{\upsilon\mathrm{e}}$ and $\nabla_{\upsilon\mathrm{h}}$.

The second term on the right in Eq. (1) describes the drift of charges due to internal fields, with $\hat{\nabla}$ denoting the 12-dimensional divergence operation and $\boldsymbol{F}$ being the drift force. This force can be obtained by correspondence with the equations of motion. It should be noted that the classical equations of motion when explicitly decomposed for electrons and holes are

$$\frac{\mathrm{d}\boldsymbol{r}_{\mathrm{e}}}{\mathrm{d}t} = \boldsymbol{\upsilon}_{\mathrm{e}}, \quad (3)$$

$$\frac{\mathrm{d}\boldsymbol{\upsilon}_{\mathrm{e}}}{\mathrm{d}t} = -\frac{e}{m_{\mathrm{e}}^{*}}\boldsymbol{E}(\boldsymbol{r}_{\mathrm{e}}), \quad (4)$$

$$\frac{\mathrm{d}\boldsymbol{r}_{\mathrm{h}}}{\mathrm{d}t} = \boldsymbol{\upsilon}_{\mathrm{h}}, \quad (5)$$

$$\frac{\mathrm{d}\boldsymbol{\upsilon}_{\mathrm{h}}}{\mathrm{d}t} = -\frac{e}{m_{\mathrm{h}}^{*}}\boldsymbol{E}(\boldsymbol{r}_{\mathrm{h}}), \quad (6)$$

where $\boldsymbol{E}(\boldsymbol{r})$ is the internal field that is present at the position of either an electron or a hole and affecting the motion of either an electron or a hole. All these fields may be expressed as gradients of the internal potential created by charged point defects. The potential energy of an electron, $U_{\mathrm{e}}(\boldsymbol{r})$, and that of a hole, $U_{\mathrm{h}}(\boldsymbol{r})$, in the presence of opposite charge and static trapped charges Q_{d} at positions $\boldsymbol{R}_{\mathrm{d}}$ is given by

$$U_{e/h}(\boldsymbol{r}) = -\chi \frac{1}{|\boldsymbol{r} - \boldsymbol{r}_{h/e}|} + \chi \sum_{d} \frac{q_{e/h} Q_d}{|\boldsymbol{r} - \boldsymbol{R}_d|}, \quad (7)$$

where the first term is due to the electron–hole interaction with $\chi = e^2/(4\pi\epsilon\epsilon_0)$ being the amplitude of the Coulomb potential, and the charge of static defect d, Q_d, is given in terms of the elementary electron charge e and $q_{e/h} = \mp 1$. The corresponding electric field affecting electrons and holes is

$$\boldsymbol{E}(\boldsymbol{r}_{e/h}) = q_{e/h} \frac{1}{2} \nabla_r U_{e/h}(\boldsymbol{r}) . \quad (8)$$

As a result, the force, which drives the probability density in the Fokker–Planck equation, is essentially given by

$$\hat{\nabla} \cdot (\rho \boldsymbol{F}) = \boldsymbol{\upsilon}_e \cdot \nabla_{re} \rho + \boldsymbol{\upsilon}_h \cdot \nabla_{rh} \rho + \frac{e}{m_e^*} \boldsymbol{E}(\boldsymbol{r}_e) \cdot \nabla_{\upsilon e} \rho - \frac{e}{m_h^*} \boldsymbol{E}(\boldsymbol{r}_h) \nabla_{\upsilon h} \rho. \quad (9)$$

Notice that here $\boldsymbol{E}(\boldsymbol{r}_e)$ includes the field induced by the hole (and not by the electron), while $\boldsymbol{E}(\boldsymbol{r}_h)$ includes the field induced by the electron (and not by the hole).

The last term in Eq. (1) is the recombination term. Assuming the homogeneous distribution of recombination centres we can define that the recombination occurs when electrons and holes meet in the space. Consequently,

$$\boldsymbol{S}(\boldsymbol{u}_e, \boldsymbol{u}_h, t) \propto \hat{\delta}(|\boldsymbol{r}_e - \boldsymbol{r}_h|). \quad (10)$$

The functions $\hat{\delta}(\epsilon)$ should not be considered as mathematical Dirac functions, instead they should be understood as distribution functions with the predefined recombination capture radius in space, σ_R. We will use the Gaussian function, the recombination radius of which is associated with the dispersion:

$$\boldsymbol{S}(\boldsymbol{u}_e, \boldsymbol{u}_h, t) \equiv S(\boldsymbol{r}_e, \boldsymbol{r}_h) = \gamma_R \exp\left(\frac{|\boldsymbol{r}_e - \boldsymbol{r}_h|^2}{2\sigma_R^2} \right). \quad (11)$$

The parameter γ_R is the on-spot recombination rate, which should be considered as the recombination rate when the wave packets of electron and hole are completely overlapping.

Combining these results we have the Boltzmann kinetic equation for the combined electron and hole density:

$$\dot{\rho} + (\boldsymbol{\upsilon}_e \cdot \nabla_{re} + \boldsymbol{\upsilon}_h \cdot \nabla_{rh}) \rho + \frac{e}{m_h^*} \boldsymbol{E}_h(\boldsymbol{r}_h) \cdot \nabla_{\upsilon h} - \frac{e}{m_e^*} \boldsymbol{E}_e(\boldsymbol{r}_e) \nabla_{\upsilon e} \rho = \left(\frac{\partial \rho}{\partial t} \right)_S + \left(\frac{\partial \rho}{\partial t} \right)_R . \quad (12)$$

The two terms on the right, i.e.

$$\left(\frac{\partial \rho}{\partial t} \right)_S = (D_e \Delta_{re} + D_h \Delta_{rh}) \rho \quad (13)$$

and

$$\left(\frac{\partial \rho}{\partial t} \right)_R = -S(\boldsymbol{r}_e, \boldsymbol{r}_h) \rho, \quad (14)$$

represent the scattering and recombination processes, respectively, which in our case are represented by diffusion and recombination rates.

3. Stochastic dynamics in the coherent regime

Complete density dynamics is conceptually very desirable; however, the size of the problem is huge. Solving the Boltzmann equation amounts to propagating electron and hole density in the 12-dimensional space. It is constructive to use a different approach, i.e. to define the problem in terms of stochastic trajectories. Notice that simple stochastic differential equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \xi_x(t), \quad (15)$$

with the initial condition $x(0) = 0$ and stochastic force properties

$$\langle \xi_x(t) \rangle = 0, \quad (16)$$

$$\langle \xi_x(t) \xi_x(s) \rangle = 2D\delta(t - s), \quad (17)$$

where D is the amplitude, generates the stochastic Brownian dynamics of x with the average $\langle x(t) \rangle = 0$, and the dispersion $\langle x(t)x(t) \rangle = 2Dt$. Such characteristics correspond to a simple diffusion equation for the probability function $\rho(x, t)$:

$$\frac{\partial \rho(x,t)}{\partial t} = D \frac{\partial^2 \rho(x,t)}{\partial x^2}, \quad (18)$$

with D being the diffusion coefficient.

In the complete semiclassical description, the fluctuating force affects the momentum of the particles and, additionally, due to the fluctuation–dissipation theorem [12], the fluctuation force induces damping. Consequently, we should consider the semiclassical equations of motion for a particle in the form of the Langevin equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \upsilon, \tag{19}$$

$$\frac{\mathrm{d}\upsilon}{\mathrm{d}t} = -\gamma\upsilon + \frac{1}{M} f + \xi_{\upsilon}(t). \tag{20}$$

The damping constant γ can be related to the particle scattering time $\gamma = \tau^{-1}$, which is available for semiconductor charges. Assuming the same conditions for the velocity-related fluctuating force,

$$\langle \xi_{\upsilon}(t) \rangle = 0, \tag{21}$$

$$\langle \xi_{\upsilon}(t)\xi_{\upsilon}(s) \rangle = 2\mathcal{D}\delta(t-s), \tag{22}$$

it can be easily shown that in the asymptotic conditions $t \gg \gamma^{-1}$ the dispersion of velocity becomes constant,

$$\langle \boldsymbol{\upsilon}(t)\boldsymbol{\upsilon}(t) \rangle = \frac{\mathcal{D}_{\mathrm{e}}}{\gamma_{\mathrm{e}}}, \tag{23}$$

while for the coordinate

$$\langle x(t)x(t) \rangle = \frac{2\mathcal{D}}{\gamma^2} t. \tag{24}$$

Accordingly, the coordinate performs the same Brownian process and the diffusion coefficients satisfy $D = \mathcal{D}/\gamma^2$.

An arbitrary 'external' drift force can be added into Eq. (20). Consider the stochastic differential equations of motion for the electron and the hole in the 3D space:

$$\frac{\mathrm{d}\boldsymbol{r}_{\mathrm{e}}}{\mathrm{d}t} = \boldsymbol{\upsilon}_{\mathrm{e}}, \tag{25}$$

$$\frac{\mathrm{d}\boldsymbol{\upsilon}_{\mathrm{e}}}{\mathrm{d}t} = -\gamma_{\mathrm{e}}\boldsymbol{\upsilon}_{\mathrm{e}} - \frac{e}{m_{\mathrm{e}}^*}\boldsymbol{E}(\boldsymbol{r}_{\mathrm{e}}) + \boldsymbol{\xi}_{\upsilon\mathrm{e}}(t), \tag{26}$$

$$\frac{\mathrm{d}\boldsymbol{r}_{\mathrm{h}}}{\mathrm{d}t} = -\boldsymbol{\upsilon}_{\mathrm{h}}, \tag{27}$$

$$\frac{\mathrm{d}\boldsymbol{\upsilon}_{\mathrm{h}}}{\mathrm{d}t} = -\gamma_{\mathrm{h}}\boldsymbol{\upsilon}_{\mathrm{h}} + \frac{e}{m_{\mathrm{h}}^*}\boldsymbol{E}(\boldsymbol{r}_{\mathrm{h}}) + \boldsymbol{\xi}_{\upsilon\mathrm{h}}(t). \tag{28}$$

The noise forces are now three-dimensional and can be described as sums of three independent noises. For electrons we have

$$\boldsymbol{\xi}_{\upsilon\mathrm{e}}(t) = \boldsymbol{x}\xi_{\upsilon\mathrm{e}}^{(x)}(t) + \boldsymbol{y}\xi_{\upsilon\mathrm{e}}^{(y)}(t) + \boldsymbol{z}\xi_{\upsilon\mathrm{e}}^{(z)}(t), \tag{29}$$

$$\langle \boldsymbol{\xi}_{\upsilon\mathrm{e}}(t) \rangle = 0, \tag{30}$$

$$\langle \xi_{\upsilon\mathrm{e}}^{(j)}(t)\xi_{\upsilon\mathrm{e}}^{(j)}(s) \rangle = 2\gamma_{\mathrm{e}}^2 D_{\mathrm{e}}\delta_{ij}\delta(t-s), \tag{31}$$

and we have the same for holes. Diffusion constants D_{e} for electrons and D_{h} for holes are defined with respect to the coordinate-related diffusion process.

These equations generate drift and diffusion processes in accordance with the Boltzmann equations. However, the recombination process cannot be embedded into the equations of motion. Instead, we add an additional equation for the probability of such pair of charges, which mimics the decay process:

$$\frac{\mathrm{d}p(t)}{\mathrm{d}t} = -S(\boldsymbol{r}_{\mathrm{e}}, \boldsymbol{r}_{\mathrm{h}})p(t). \tag{32}$$

By adding this equation, we find the complete stochastic description of the system dynamics, which is equivalent to Eq. (12).

A large number of trajectories are required to reconstruct the multidimensional density function. Their statistical ensemble generates the complete distribution function

$$\rho(\boldsymbol{\upsilon}_{\mathrm{e}}, \boldsymbol{\upsilon}_{\mathrm{h}}, \boldsymbol{r}_{\mathrm{e}}, \boldsymbol{r}_{\mathrm{h}}, t) = \sum_i p^{(i)}(t)\delta(\boldsymbol{\upsilon}_{\mathrm{e}} - \boldsymbol{\upsilon}_{\mathrm{e}}^{(i)}(t))\,\delta(\boldsymbol{\upsilon}_{\mathrm{h}} - \boldsymbol{\upsilon}_{\mathrm{h}}^{(i)}(t)) \\ \delta(\boldsymbol{r}_{\mathrm{e}} - \boldsymbol{r}_{\mathrm{e}}^{(i)}(t))\delta(\boldsymbol{r}_{\mathrm{h}} - \boldsymbol{r}_{\mathrm{h}}^{(i)}(t)). \tag{33}$$

Here i labels the independent trajectory, consisting of the set ($\boldsymbol{r}_{\mathrm{e}}^{(i)}(t)$, $\boldsymbol{\upsilon}_{\mathrm{e}}^{(i)}(t)$, $\boldsymbol{r}_{\mathrm{h}}^{(i)}(t)$, $\boldsymbol{\upsilon}_{\mathrm{h}}^{(i)}(t)$, $p^{(i)}(t)$). However, it is not necessary to store all this information. If we are interested only in recombination kinetics, it is sufficient to follow the function

$$n(t) = \frac{1}{N}\sum_i^N p^{(i)}(t), \tag{34}$$

which is just a one-dimensional function.

4. Overdamped case

The coherent dissipative dynamics of an electron and a hole described in the previous section should

be considered when the particle damping is relatively small compared to drift forces, or $\dot{v}_i \gg \gamma_i v_i$, where i = e, h. In the recent study, the coherent dynamics was neglected by considering only the overdamped regime, which corresponds to the opposite inequality $\dot{v}_I \ll \gamma_i v_i$. Then taking $\frac{\mathrm{d}v_\mathrm{e}}{\mathrm{d}t} = 0, v_i$ can be plugged into the coordinate equation that yields the reduced set of the equations of motion for the coordinates:

$$\frac{\mathrm{d}\boldsymbol{r}_\mathrm{e}}{\mathrm{d}t} = -\frac{}{m_\mathrm{e}^*\gamma_\mathrm{e}}\boldsymbol{E}(\boldsymbol{r}_\mathrm{e}) + \boldsymbol{\xi}_\mathrm{e}(\ ), \tag{35}$$

$$\frac{\mathrm{d}\boldsymbol{r}_\mathrm{h}}{\mathrm{d}t} = \frac{e}{m_\mathrm{h}^*\gamma_\mathrm{h}}\boldsymbol{E}(\boldsymbol{r}_\mathrm{h}) + \boldsymbol{\xi}_{r\mathrm{h}}(t), \tag{36}$$

$$\frac{\mathrm{d}p(t)}{\mathrm{d}t} = -S(\boldsymbol{r}_\mathrm{e}, \boldsymbol{r}_\mathrm{h})\,p(t). \tag{37}$$

Now $\boldsymbol{\xi}_{re/h}(t)$ is the three-dimensional coordinate-related fluctuating 'force' in the form of Eq. (17). As a result, we can construct the coordinate-only distribution function

$$\rho(\boldsymbol{r}_\mathrm{e}, \boldsymbol{r}_\mathrm{h}, t) = \sum_i p^{(i)}(t)\,\delta(\boldsymbol{r}_\mathrm{e} - \boldsymbol{r}_\mathrm{e}^{(\mathrm{i})}(t))\,\delta(\boldsymbol{r}_\mathrm{h} - \boldsymbol{r}_\mathrm{h}^{(i)}(t)). \tag{38}$$

The combined probability density also defines separate electron and hole distributions. The electron distribution function is obtained by integrating out the hole variables,

$$\rho_\mathrm{e}(\boldsymbol{r}_\mathrm{e}, t) = \int_V \mathrm{d}^3\boldsymbol{r}_\mathrm{h}\,\rho(\boldsymbol{r}_\mathrm{e}, \boldsymbol{r}_\mathrm{h}, t), \tag{39}$$

and similarly for the hole distribution function,

$$\rho_\mathrm{h}(\boldsymbol{r}_\mathrm{h}, t) = \int_V \mathrm{d}^3\boldsymbol{r}_\mathrm{e}\,\rho(\boldsymbol{r}_\mathrm{e}, \boldsymbol{r}_\mathrm{h}, t), \tag{40}$$

while the total probability of an electron and a hole being in the system is given by

$$n(t) = \int_V \mathrm{d}^3\boldsymbol{r}_\mathrm{h} \int_V \mathrm{d}^3\boldsymbol{r}_\mathrm{e}\,\rho(\boldsymbol{r}_\mathrm{e}, \boldsymbol{r}_\mathrm{h}, t). \tag{41}$$

These functions satisfy the overdamped case of the Boltzmann kinetic equation [13]:

$$\dot{\rho}_\mathrm{e}(\boldsymbol{r}, t) = D_\mathrm{e}\Delta\rho_\mathrm{e}(\boldsymbol{r}, t) - \bar{R}\frac{\rho_\mathrm{h}(\boldsymbol{r}, t)\rho_\mathrm{e}(\boldsymbol{r}, t)}{n(t)} - \frac{e}{m_\mathrm{e}^*\gamma_\mathrm{e}}\boldsymbol{E}_\mathrm{e}(\boldsymbol{r})\cdot\nabla\rho_\mathrm{e}(\boldsymbol{r}, t), \tag{42}$$

$$\dot{\rho}_\mathrm{h}(\boldsymbol{r}, t) = D_\mathrm{h}\Delta\rho_\mathrm{h}(\boldsymbol{r}, t) - \bar{R}\frac{\rho_\mathrm{h}(\boldsymbol{r}, t)\rho_\mathrm{e}(\boldsymbol{r}, t)}{n(t)} - \frac{e}{m_\mathrm{h}^*\gamma_\mathrm{h}}\boldsymbol{E}_\mathrm{h}(\boldsymbol{r})\cdot\nabla\rho_\mathrm{h}(\boldsymbol{r}, t), \tag{43}$$

with $\bar{R}$ being the average on-site recombination rate.

The electron and hole distribution functions are again related to the sum over stochastic trajectories:

$$\rho_\mathrm{e}(\boldsymbol{r}, t) = \sum_i p^{(i)}(t)\delta(\boldsymbol{r} - \boldsymbol{r}_\mathrm{e}^{(i)}(t)), \tag{44}$$

$$\rho_\mathrm{h}(\boldsymbol{r}, t) = \sum_i p^{(i)}(t)\delta(\boldsymbol{r} - \boldsymbol{r}_\mathrm{h}^{(i)}(t)). \tag{45}$$

Following the time evolution of

$$n(t) = \int_V \mathrm{d}^3\boldsymbol{r}_\mathrm{h}\rho_\mathrm{h}(\boldsymbol{r}_\mathrm{h}, t) \equiv \int_V \mathrm{d}^3\boldsymbol{r}_\mathrm{e}\rho_\mathrm{e}(\boldsymbol{r}, t), \tag{46}$$

allows one to define the rate of recombination characteristic of the system.

5. Results

Below we present the application of the stochastic theory to the electron and hole dynamics in the bulk Si crystal affected by defect clusters. The bulk parameters are considered as follows. The presented theory does not include the electron–electron and hole–hole interaction, hence we denote this as the single-particle approximation. Assuming that at ambient conditions the concentration of charges is ~10^{15} cm^{-3}, we obtain that a cubic box with 100 nm edge length would contain a single electron and a single hole. Consequently, we consider such cube as a sample. To start, we generate an electron and a hole at random locations in this box and propagate them according to the equations of motion. As they move and reach either side of the box, they are translated to the opposite side, and that reflects the 'old' particle departure and the 'arrival' of a new particle. Hence particle positions always change and we obtain the required electron and hole concentrations. For effective masses we take the longitudinal electron at the conduction band minimum, $m^*_\mathrm{e} = 0.98\ m_\mathrm{e}$, where m_e is the electron mass. Two types of holes can be taken into account with a different set of parameters: a heavy hole, $m^*_\mathrm{hh} = 0.49\ m_\mathrm{e}$, and a light hole, $m^*_\mathrm{lh} = 0.16\ m_\mathrm{e}$, corresponding to different energy bands. Given the effective mass,

the particle relaxation time is obtained from the mobility relation $\mu_{e/h} = e\tau_{e/h}/m^*_{e/h}$, where e is the electron charge. The corresponding coherence decay rate $\gamma_{e/h} = \tau^{-1}_{e/h} = e/(\mu_{e/h}m^*_{e/h})$. The Einstein relation $D_i = \mu_i k_B T$ defines the diffusion constant and mobility and, consequently, we have $\tau_{e/h}/m^*_{e/h} = \mu_{e/h}/e$ irrespective of the effective mass. We then use experimental mobility values, $\mu_e = 1400$ cm^2/(Vs) and $\mu_h = 450$ cm^2/(Vs), and the corresponding diffusion constants, $D_e = 36$ cm^2/s and $D_h = 12$ cm^2/s. Additionally, the Coulomb field is scaled by the Si dielectric constant $\epsilon = 11.68$. The recombination process is characterized by the on-spot event when the electron and the hole encounter at the same space and is characterized by Eq. (11). We assume that the on-spot recombination is fast with $\gamma^{-1}_R = 1$ ps and the recombination radius $\sigma_R = 5$ nm. These are essentially free parameters of the model and can be fitted to some experiments. Time step of 0.1 fs is used for the integration of equations. Also, for numerical stability the Coulomb interaction potential is shifted by $\eta = 5$: $1/r \to 1/\sqrt{x^2 + y^2 + z^2 + \eta^2}$.

As a starting position, we consider a homogeneous distribution of electrons and holes. In Fig. 1, we present the calculated free electron and hole trajectories in the coherent and overdamped cases for 10 ps time interval in the pure system. It is important to note that during this time recombination is practically absent. This corresponds to the notion that recombination in a clean sample is very slow. However, Fig. 2 presents the importance of coherence in the electron description. The hole dynamics can be described using the overdamped regime. Only a small difference between the light hole and the heavy hole is noticed.

In order to properly describe the recombination process in the presence of defects, it becomes imperative to include additional recombination centres. Stochastic description allows one to include trapping of charges by specific trapping/recombination centres. Assuming that the concentration of such trapping centres is $\sim 10^{16}$ cm^{-3} we find that there are about 10 trapping centres in the (100 nm)^3 cube. Assuming homogeneous conditions, their positions within the cube are chosen randomly using the uniform distribution in the 3D space. They are then characterized by the electron and hole capture radius $R_c = 5$ nm: so if an electron or a hole appears at a distance smaller than R_c to any trapping centre, they become trapped in space

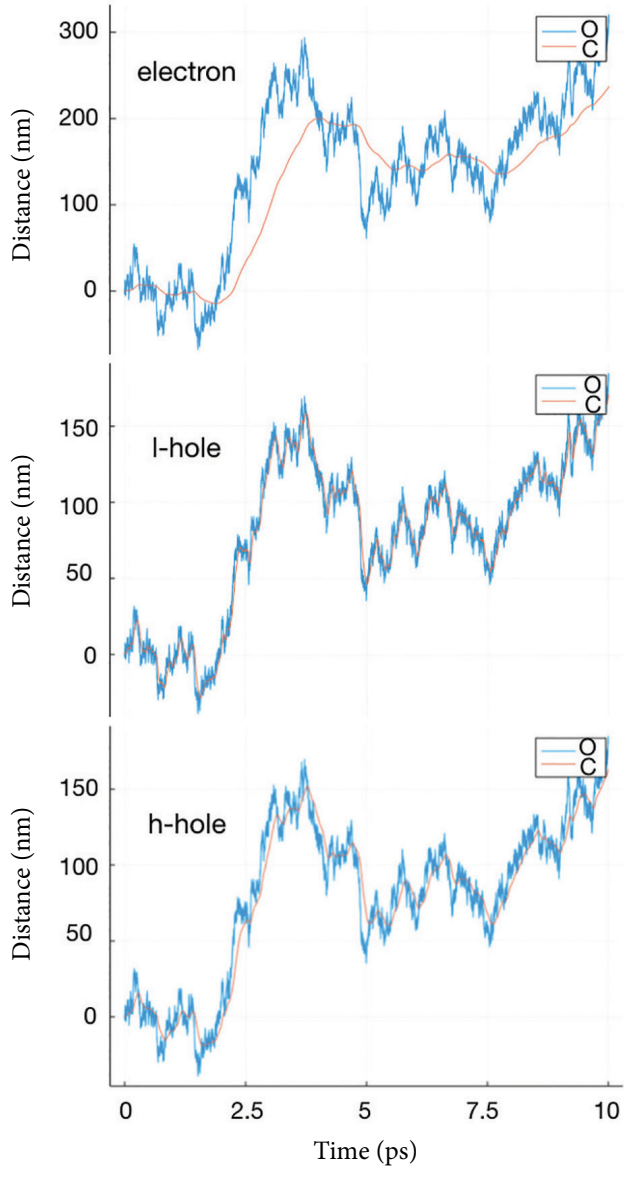

Fig. 1. Free electron and hole trajectories (l denotes light, h denotes heavy) in the coherent (C) and overdamped (O) cases for 10 ps time interval in the pure system.

for the time t_C (i.e. their motion is stopped for that time interval). At room temperature, the trapped charges can be thermally activated and detrapped. The detrapping process is statistical, even having exponential statistics, i.e. the probability of being trapped decays in time as $\exp(-t_C/\bar{t}_C)$, so that t_C is distributed exponentially. It is assumed that the detrapping average time is $\bar{t}_C = 10$ ps. As the charge becomes detrapped, it moves again according to the stochastic equations of motion.

The recombination kinetics calculated using such conditions is presented in Fig. 2. Decay kinetics in all cases is almost exponential. The coherent

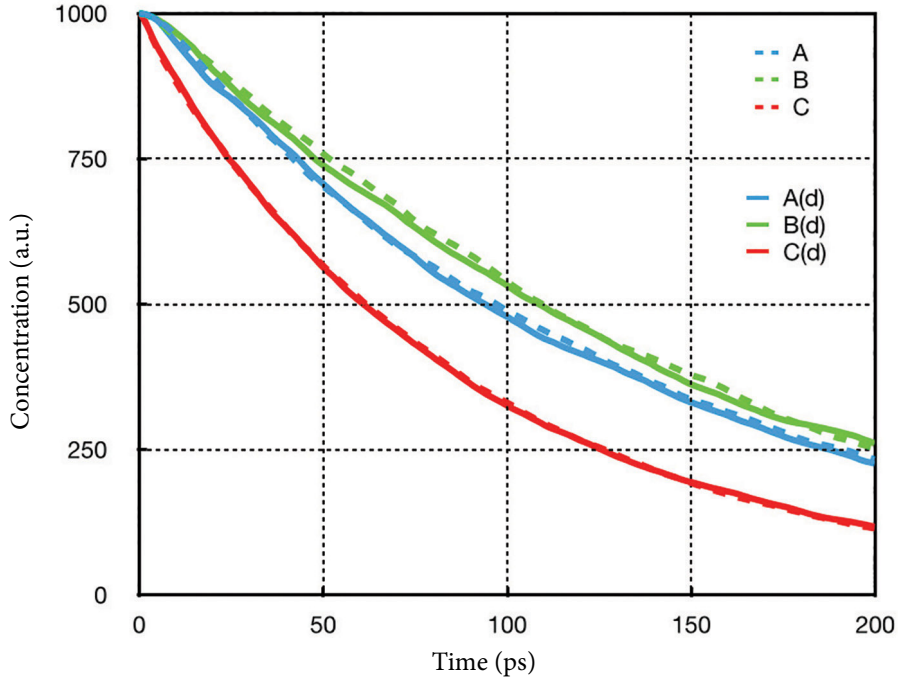

Fig. 2. Charge recombination kinetics: A, the coherent model with a heavy hole; B, the coherent model with a light hole; C, the overdamped model. Dashed line: no static dipole; solid line: with the dipole present, indicated by (d).

model using the heavy hole shows the slowest decay curve with the decay time 142 ps (this number is obtained by exponential curve fitting). The light hole case gives slightly faster decay kinetics with 135 ps decay time. An identical setup, while using the overdamped model gives faster decay kinetics with the 100 ps decay time. Consequently, the overdamped model is not the perfect approximation and the error is introduced. There is no difference between using light holes or heavy holes in the overdamped case – the mass of the hole directly influences only coherence hole dynamics, so the overdamped regime is not depending on masses of particles. Overall, the result is that the trapping centres influence considerably recombination kinetics. They essentially enable the recombination process.

It has been proposed that the inhomogeneous distribution of defects may result in static internal electric fields, created by permanently trapped charges [8, 13, 14]. In the overall neutral system, the lowest multipole moment is the dipole moment. Consequently, the dipolar electric field shall be considered to mimic the inhomogeneous configuration defects. Two static charges of $Q = \pm e$ are placed at positions ±20 nm along the z direction from the centre of the box. It corresponds to the scenario that one electron and one hole are permanently trapped at these positions. Using these conditions we have calculated the charge recombination kinetics for different models. Figure 2 case A(d) presents the charge recombination kinetics using the coherent model with the heavy hole. The recombination process becomes slightly faster in the first 100 ps time interval. Later the process becomes similar to the case without the static trapped dipole. However, there is no considerable effect on the dynamics for the light hole and for the overdamped simulations.

6. Discussion and conclusions

Charge dynamics simulation approaches based on the semiclassical approximation have been developed and applied to describe charge recombination in the vicinity of defect clusters. The approach corresponds to the Boltzmann equation theory. Developed in the form of stochastic trajectories, the methods contain a number of advantages. First, the stochastic theory is much more computationally acceptable, since there is no need to solve the 12-dimensional distribution of electron and hole density. The density can be reconstructed from stochastic trajectories – they can be run in parallel on a supercomputer, so a large number of trajectories can

be generated independently. Second, the theory is also very flexible as both coherent and overdamped regimes are easily achievable. Third, additional various local trapping/recombination sites or recombination centres can be added. The fourth and the most important advantage compared to other very popular Monte Carlo hopping approach is that the space does not need to be broken into an artificial discrete lattice. The continuous space is used instead. Consequently, the numerically very efficient theory with overlapping properties of different types of defects is easily organized.

The presented flexible theory allows one to determine several important observations. It should be noted that our previous calculations, based on probability density [13], considered only the overdamped regime. In the present study, the coherent regime was additionally considered. This gives two distinct qualitative features: (i) it dramatically affects the electron evolution, and (ii) considerably changes the dynamics of light holes. It has to be noted that only the heavy hole can be described in the complete overdamped regime. However, switching between the overdamped and complete coherent regime makes (especially electron) dynamics much less fluctuating and thus the recombination becomes slower. Electron dynamics on the longer scale covers the same area in both coherent and overdamped regimes; however, the extent of small-scale fluctuations is much larger in the overdamped regime. While the introduced errors are not dramatic, the numerical values are affected. As a result, the electron dynamics cannot be described in the overdamped regime in bulk Si.

The previous analysis of electronic parameters revealed that the most significant parameter describing charge evolution and recombination in the defect cluster is the diffusion coefficient [13]. Values of diffusion coefficients for electrons and holes are large enough so that electrons cover 600 nm per 100 ps. The hole covers a smaller distance, while it is still considerably larger than the size of the cube under consideration. Using periodic boundary conditions we get the result that the particles cross the cube many times in a simulation window of 200 ps. This is actually a positive feature, which mimics the fact that the number of electrons and holes is large. Assuming the average charge concentration of 10^{15} cm^{-3}, we have that there is one electron and one hole in a cube of 100 nm linear extension. As a result, the Coulomb interactions make a secondary effect, while charge dynamics in the studied conditions is almost free.

However, this study of a single dipolar internal field is applied when defect concentration is relatively low. If the defect concentration is high, the internal fields are no more dipolar and bulk properties like mobility, diffusion constant and effective masses may be extensively affected. As the parameters become different, the eventual recombination rate can be strongly affected, but hardly characterizable.

In the present simulations, we thus find that the most significant factor influencing the recombination process is related to the appearance of electron and hole trapping centres. They indeed slow down electron and hole diffusion and thus effectively increase the chances of the electron to meet holes. In the pure system (without trapping centres), the probability of the electron and the hole to be in the same volume v when the considered box volume is V is equal to the ratio v/V. By taking the box size of 100 nm and the recombination capture radius 5 nm we find that the probability is equal to 10^{-4}. Hence by using the 'on the spot' recombination time of 1 ps we find that in the pure system in these conditions the recombination time becomes 10^4 larger, i.e. 10 ns, which is a proper parameter for the bulk. However, introducing trapping centres (defects) we speed up the process considerably, and consequently, locally in the vicinity of defect cluster with a large amount of various defects the recombination becomes much faster – this is properly described by the theory.

As already described, additional internal electric fields become secondary effects. Essentially, they make quite a small effect on recombination kinetics.

Concluding, we have presented the theoretical analysis of charge recombination in the Si crystal in the vicinity of trapped charge creating dipolar field using the stochastic coherent modelling, corresponding to the Boltzmann equation. We find that electron dynamics is very roughly described in the overdamped regime and the coherent regime is a much better approach. Additionally, the local trapping centres for mobile charges create the necessary conditions for the fast charge recombination.

Additional internal electric fields make a small contribution to the process.

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STOCHASTINĖ KRŪVININKŲ DINAMIKOS IR REKOMBINACIJOS SILICYJE TEORIJA

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Santrauka

Silicio pagrindu sukurtuose elektringų dalelių detektoriuose didelės energijos spinduliuotė sukuria daugybę taškinių defektų, kurie yra laisvųjų krūvininkų pagavimo ir rekombinacijos centrai. Užpildyti pagavimo centrai sukuria vidinius elektrinius laukus, kurie gali daryti įtaką laisvųjų krūvininkų dinamikai bei jų rekombinacijos charakteristikoms. Norint įvertinti skirtingų reiškinių įtaką rekombinacijos spartai, buvo atliktas kompiuterinis elektronų ir skylių dinamikos modeliavimas. Pusiau klasikiniame modelyje krūvininkų dinamika aprašoma Bolcmano lygtimi. Šiame straipsnyje naudojamas alternatyvus stochastinis modelis, kuris yra Bolcmano lygties atitikmuo, tačiau paprasčiau realizuojamas kompiuteriniais modeliavimo metodais. Be to, stochastiniame modelyje paprasta įtraukti pagavimo ir rekombinacijos centrus. Skaičiavimais parodoma, kad skylių dinamika gerai aprašoma, naudojant nuslopintos dinamikos artinį, kai inerciniai reiškiniai neįskaitomi. Elektronų dinamika turi būti aprašoma įskaitant inercinius narius. Parodoma, kad vidiniai elektriniai laukai daro silpną įtaką rekombinacijos kinetikoms, o esminis dalykas yra tiesiog rekombinacijos centrų tankis.