BASIC KINETIC MODEL FOR X-RAY CONDUCTIVITY IN WIDE-GAP SEMICONDUCTORS

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A logical scheme for the development of a basic kinetic theory of X-ray conductivity in semiconductors has been proposed. It includes the calculation of spatial distributions of free charge carriers at successive time moments and uses the model of diffusion-driven drift motion of free charge carriers in a solid. An analytic expression for the basic shape of a current pulse in the external circuit has been obtained in the case of ideal semiconductor, i.e., when it does not contain deep traps and recombination centers. Basic dependences of the current pulse shape on the coordinate of an X-ray quantum absorption event and the strength of an applied electric field have been obtained.

1. Introduction

Nowadays, semiconductor materials are widely used in ionizing radiation detectors. The advantage of semiconductor detectors (SCDs) over other sensor systems (scintillation and tracking ones) consists in a direct transformation of the ionizing radiation energy into an electric current, which allows them to be successfully used in spectrometry researches. In this case, an important criterion of the detector quality is the charge collection efficiency at the registration of an individual ionizing particle or a quantum [1–5], because even small charge losses of several percent at the charge drift make the line shape in a detector response function much more complicated [5–7]. Unfortunately, the modern approaches to the calculation of the charge collection dynamics in SCDs [5–8] do not consider the influence of the thermal velocity of charge carriers on the kinetics of their drift, although the thermal velocity still prevails over the drift one even if the SCDs are cooled down to temperatures of about 150 K. This circumstance has to be taken into consideration in the theoretical analysis of the processes of charge collection and current pulse formation in the external electric circuit of a detector.

All physical processes that take place at the drift of charge carriers in SCDs are known, but there is the lack of a general kinetic model for their quantitative calculation. The construction of such a model should be started from the consideration of the most simplified physical scenario, which should be gradually—step by step—made more and more complicated, approaching the real picture. The consideration should also be started from such ionizing radiation that does not create new structural defects in the detector material. Proceeding from those conditions, the analysis should be started from the development of a kinetic model for X-ray conductivity (XRC) in an ideal semiconductor crystal without recombination and trapping centers. Knowing the dependence of the current pulse shape on the diffusion-drift parameters of the charge carrier motion, the next step – the consideration of the influence of shallow and deep traps on the current pulse and the charge collection efficiency (and, hence, on the detector response function) – can be done.

2. Model for X-ray Conductivity Kinetics

X-ray conductivity appears, when X-ray quanta are absorbed. The corresponding mechanisms of electron-hole pair generation and the initial average distribution of electron-hole pairs in space at the generation stage were studied in detail in the framework of the kinetic theory of X-ray luminescence (XRL) [9, 10]. It should be noted that the trajectories of individual high-energy electrons, which arise when X-ray quanta are absorbed, are not identical but statistically random. Therefore, for the consideration of XRL and XRC, the concept of "aver-

age spatial distribution of electron excitations" has been introduced for charge carriers in space [10].

In experimental XRL and XRC researches, plenty of exciting quanta (more than 10^6) absorbed non-uniformly in the substance are always used. The absorption of X-ray radiation is governed by the Bouguer–Lambert law. Similarly to what happens at photoexcitation, X-ray radiation creates macroscopically non-uniform electron excitations in a crystal. However, unlike photoexcitation, the absorption of X-ray quanta is accompanied by the generation of hundreds of thousands of charge carriers. That is why X-ray irradiation gives also rise to the appearance of a local microscopic non-uniformity of excitation. The kinetics of luminescence and conductivity has to take such local microscopic non-uniformities into account in this case. In work [11], the conductivity and luminescence of wide-gap semiconductors were experimentally confirmed to depend substantially on the excitation type. However, such differences cannot be explained in the framework of classical kinetic equations [12, 13].

The physical aspects of motion of free charge carriers were studied in detail in the kinetic theory of photoconductivity (PC) and the semiconductor theory [12–16]. They can be applied to studying the XRC as well. For the construction of a kinetic model of XRC, it is necessary to firstly consider, in detail, the kinetics of motion of free charge carriers generated at the absorption of one X-ray quantum. To build a basic XRC model, let us consider only the main processes. We use the following assumptions:

1. The energy of an X-ray quantum is insufficient for the creation of new structural defects in the detector material.

2. Free charge carriers are generated in a very small volume of a semiconductor [10]. The number of generated pairs N_0 is determined by the energy of an X-ray quantum, $h\nu_X$, and the energy gap width in the semiconductor, E_g [17]: $N_0 = \frac{h\nu_X}{3E_g}$.

3. The initial spatial distributions of electrons and holes are identical.

4. The electric field in a semiconductor is uniform. It is determined by the potential difference applied to the electric contacts and the specimen thickness.

5. The local region of free carrier generation at the absorption of an X-ray quantum is cooled down within several tens of picoseconds in almost all semiconductors [9]. This allows the local heating at the absorption of an X-ray quantum to be neglected.

Since the rates of various XRC processes are different, the general XRC kinetics can be actually separated in time into three basic stages:

1. The generation stage ($t = 0 \div 10^{-12}$ s), during which an X-ray quantum is absorbed, and a high-energy photoelectron emerges. The photoelectron generates, at the thermalization, an initial average spatial distribution of N_0 free electrons and P_0 free holes ($N_0 = P_0$).

2. The migration stage ($t = 10^{-12} \div 10^{-7}$ s), when the spatial distribution of free charge carriers changes owing to their diffusion-drift motion (localization of carriers at probable recombination centers and traps; delocalization of carriers from shallow traps, followed by the charge collection at electrodes). The complete calculation of this stage allows the amplitude and the shape of a current pulse in the external circuit at the absorption of one X-ray quantum to be determined.

3. The relaxation stage ($t > 1$ s) includes the delocalization of charge carriers from deep traps. The carriers can be localized again at the recombination centers or traps. Alternatively, under the action of an external field, they reach contacts with a large time lag. In other words, they can create a practically constant background current.

The time boundaries between stages are rather relative, so that the stage periods can vary even by several orders of magnitude, depending on the semiconductor substance, electric field strength, and specimen thickness. Such a classification of stages allows the calculations to be simplified considerably, because only a few processes dominate at each stage.

The following logic scheme can be used to construct the kinetics of X-ray conductivity. First, it is necessary to determine the shape of a current pulse in the external circuit at the absorption of one X-ray quantum in an ideal semiconductor, i.e. when the latter does not contain traps and recombination centers. Such a pulse shape will serve a reference point for the further account of centers of various types which will change this pulse. Then, it is necessary to take the Coulomb interaction between free carriers with opposite charge signs into account. Afterwards, point defects may be introduced into the consideration: first, shallow traps; then deep traps and recombination centers. The introduction of point defects into the calculation scheme will allow the variation kinetics of free carrier spatial distributions to be established and, accordingly, a variation of the current pulse shape to be found. Knowing the shape of a current pulse that arises in the external circuit, when an X-ray quantum is absorbed, one can calculate the charge collection efficiency as well. The summation of separate

pulses will allow the total current of X-ray conductivity to be determined.

3. Generation of Free Charge Carriers and Their Motion

When an X-ray quantum with an energy of 1 to 50 keV interacts with a solid, the main process is the photoabsorption of the quantum, resulting in the emergence of both an ion in the solid and a high-energy photoelectron. The photoelectron, due to ionization losses of its kinetic energy in the course of thermalization ($10^{-13} - 10^{-12}$ s), creates N_0 electron-hole pairs, on the average, in a local volume. Using the diffusion model for the photoelectron thermalization process [10], one can obtain the average spatial distribution of the concentration of generated free charge carriers $N_0(r)$, which is well described by the Gaussian distribution:

$$N_0\,(r) = \frac{N_0}{(2\pi)^{3/2}\ r_g^3} \exp\left(-\frac{r^2}{2r_g^2}\right), \tag{1}$$

where r_g is the generation stage parameter which is determined unambiguously in terms of the substance parameters and the energy of X-ray quantum [10]. Such a spatial distribution of free electrons and holes can be accepted as initial for the following migration stage. The charge carriers generated within the time interval of about $10^{-12} - 10^{-11}$ s become thermalized [16] due to their interaction with crystal lattice phonons.

4. Spatial Distribution of Charge Carriers at Their Drift

An external electric field and the concentration gradient of generated charge carriers in the crystal invoke the drift and diffusion currents, the density of which is determined in the general case by the relation

$$\mathbf{J}^{\pm} = eN^{\pm}(x,y,z,t)\cdot\mu^{\pm}\mathbf{E} \mp eD^{\pm}\boldsymbol{\nabla}N^{\pm}(x,y,z,t). \tag{2}$$

The sign "+" in Eq. (2) corresponds to holes, and the sign "–" to electrons, $N^{+}(x,y,z,t)$ and $N^{-}(x,y,z,t)$ are the spatial concentration distributions of generated free carriers with the corresponding sign, $\mathbf{E}$ is the electric field vector, $D^{\pm}$ are the diffusion coefficients of charge carriers, and $\mu^{\pm}$ are their mobilities. To be unambiguous in the choice of a charge carrier drift direction, consider a Cartesian coordinate system, in which the OX axis is normal to the detector electrodes and opposed to the electric field direction. Relation (2) in the accepted coordinate system should be appended by the continuity equation for the time-variation of the charge carrier concentration. Together, they allow one to obtain a system of kinetic equations for the diffusion-drift motion of electrons and holes:

$$\begin{cases} \dfrac{\partial N^{-}}{\partial t} = D^{-}\,\Delta N^{-} - \mu^{-}\,\mathbf{E}\,\boldsymbol{\nabla}N^{-}\,, \\ \dfrac{\partial N^{+}}{\partial t} = D^{+}\,\Delta N^{+} + \mu^{+}\,\mathbf{E}\,\boldsymbol{\nabla}N^{+}\,. \end{cases} \tag{3}$$

We suppose the dimensions of a local region, where free charge carriers are generated, to be much less than the detector thickness d, and the transverse dimensions of the detector (along the directions OY and OZ) to be much larger than its thickness. This allows the delta-function approximation to be used as the initial distribution of charge carriers, because the parameter r_g in Eq. (1) is much smaller than the dimensions of the drift region in SCDs. Having achieved the electrodes, the charge carriers disappear from the total distribution. Therefore, the following boundary conditions must be applied, when solving the system of equations (3):

$$\begin{cases} N^{+}(0,y,z,t) = N^{-}(0,y,z,t) = 0, \\ N^{+}(d,y,z,t) = N^{-}(d,y,z,t) = 0. \end{cases} \tag{4}$$

The solution of Eqs. (3) determines the spatial concentration distribution of charge carriers at their drift. It can be obtained using the variable separation method:

$$N^{\pm}(x,y,z,t) = \frac{N_0}{4\pi D^{\pm}\,t}\exp\left[-\frac{(y-y_0)^2+(z-z_0)^2}{4D^{\pm}\,t}\pm\right.$$

$$\left.\pm\frac{\mu^{\pm}E\,(x-x_0)}{2D^{\pm}} - \frac{(\mu^{\pm}E)^2 t}{4D^{\pm}}\right] \times \frac{2}{d}\sum_{n=1}^{\infty}\left\{\sin\left(\frac{\pi n x}{d}\right)\times\right.$$

$$\left.\times\sin\left(\frac{\pi n x_0}{d}\right)\,\exp\left[-\left(\frac{\pi n}{d}\right)^2 D^{\pm}\,t\right]\right\}, \tag{5}$$

where x_0 is the coordinate of an X-ray quantum absorption event in a semiconductor. In Fig. 1, the calculated distribution functions for the concentration of free electrons along the OX direction in a silicon detector at various time moments are depicted. At calculations, we used the data on the mobility of charge carriers in Si taken from work [17].

5. Current Pulse Shape at X-ray Conductivity

To calculate the current $i(t)$ created by generated free charge carriers (q^{-} and q^{+}) in the external electric circuit at their drift to electrodes under the action of an

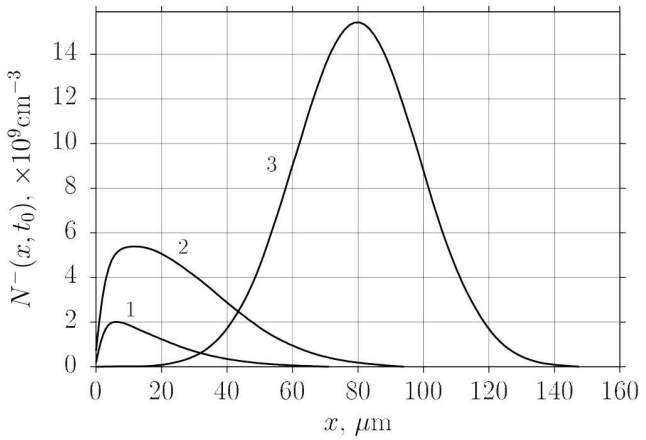

Fig. 1. Spatial distributions of electrons along the OX direction in a flat Si crystal at various time moments $t = 125$ (*1*), 100 (*2*), and 50 ns (*3*). Calculation parameters are $d = 300$ μm, $x_0 = 150$ μm, $E = 100$ V/cm, and $T = 300$ K

electric field $E = U/d$, it is necessary to apply the Ramo–Shockley theorem for point-like charges [20, 21]. Since the work done by the electric field to move all free charge carriers is defined as a sum of works done to move every carrier, the current in the external circuit is determined as a sum of currents created by every free charge carrier:

$$i(t) = \frac{q^-(t)\,\mu^- E}{d} + \frac{q^+(t)\,\mu^+ E}{d} =$$

$$= \frac{eN_0E}{d}\left[E(t)\,\mu^- + P(t)\,\mu^+\right], \qquad (6)$$

where $E(t)$ and $P(t)$ are the fractions of those generated electrons and holes, respectively, which remain free at the time moment t and continue to drift. This relation is valid for a uniform electric field and in the case where the resistance of the external electric circuit of a detector can be neglected (the corresponding scheme of XRC current measurement is shown in Fig. 2). Using relation (5), one can obtain the relative numbers of free charge carriers of each sign, $E(t)$ and $P(t)$, at every time moment:

$$E(t) = \frac{1}{N_0}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{0}^{d} N^-(x,y,z,t)\,dx\,dy\,dz\,,$$

$$P(t) = \frac{1}{N_0}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty}\int\limits_{0}^{d} N^+(x,y,z,t)\,dx\,dy\,dz\,. \qquad (7)$$

In Fig. 3, the calculated dependences of relative values of a charge collected at Si-detector electrodes in the

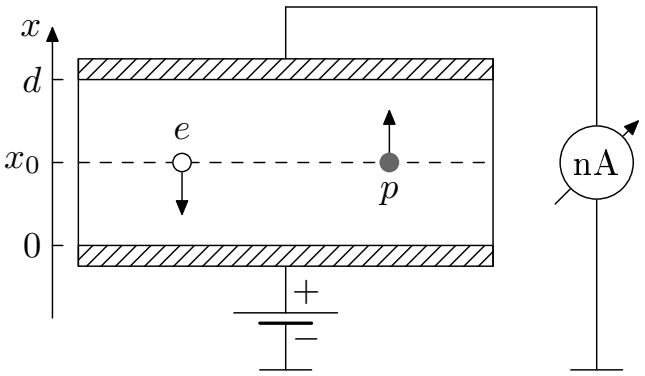

Fig. 2. Measurement scheme for the X-ray conductivity current in a semiconductor detector

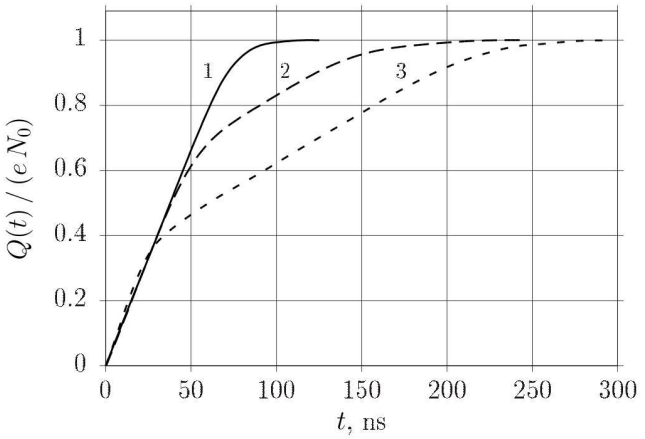

Fig. 3. Kinetics of the relative charge collection on Si-detector electrodes at the charge carrier drift calculated for various registration coordinates: 150 (*1*), 100 (*2*), and 50 μm (*3*). Calculation parameters are $d = 200$ μm, $E = 140$ V/cm, and $T = 300$ K

cases where charge carriers are generated at various detector points are depicted. They testify to a considerable influence of free carrier mobilities on the current pulse duration. In Fig. 4, the results of calculations of the current pulse shape in a Si-detector at various electric field strengths are shown. The prolonged damping of the calculated current pulse amplitudes results just from the diffusion-driven expansion of the spatial distribution of carriers at their drift.

The solution of Eqs. (7) becomes considerably complicated due to the fact that expression (5) includes an infinite series. The calculations can be simplified to some extent, if one takes into account that the relation $\frac{\mu^{\pm}Ed}{2D^{\pm}} \gg 1$ is practically always satisfied. Then Eqs. (7), after integration, can be expressed in the following sim-

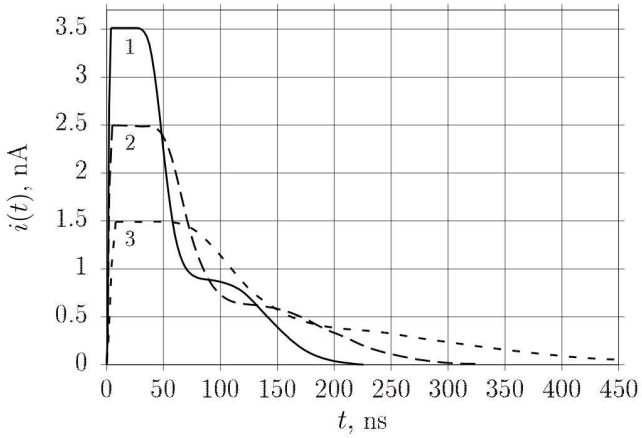

Fig. 4. Current pulse shapes in a Si-detector at various electric field strengths $E = 140$ (*1*), 100 (*2*), and 60 V/cm (*3*). Calculation parameters are $d = 200$ μm, $x_0 = 100$ μm, and $T = 300$ K

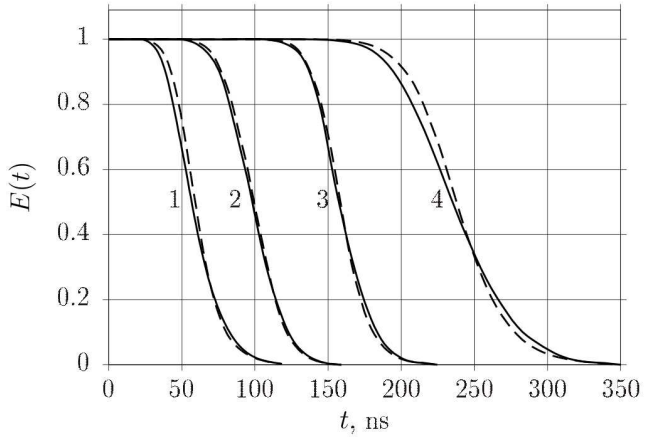

Fig. 5. Exact theoretical function $E(t)$ (solid curves) and its approximation (dash-dotted curves) for various registration coordinates x_0 and electric fields E in a ZnSe-based detector: (*1*) $x_0 = 50$ μm, $E = 120$ V/cm; (*2*) $x_0 = 125$ μm, $E = 180$ V/cm; (*3*) $x_0 = 200$ μm, $E = 180$ V/cm; and (*4*) $x_0 = 200$ μm, $E = 120$ V/cm. Calculation parameters are $d = 250$ μm and $\mu^- = 700$ cm^2/(V × s)

plified form:

$$E(t) = \frac{2}{\pi}\exp\left[\frac{\mu^- E}{4D^-}(2x_0 - \mu^- E\,t)\right] \times$$

$$\times \sum_{n=1}^{\infty}\left\{\frac{n\,\exp\left[-\left(\frac{\pi n}{d}\right)^2 D^- t\right]\sin\left(\frac{\pi n x_0}{d}\right)}{\left(\frac{\mu^- E\,d}{2\pi D^-}\right)^2 + n^2}\right\},$$

$$P(t) = \frac{2}{\pi}\exp\left\{\frac{\mu^+ E}{4D^+}[2(d - x_0) - \mu^+ E\,t]\right\} \times$$

$$\times \sum_{n=1}^{\infty}\left\{\frac{(-1)^n\,n\,\exp\left[-\left(\frac{\pi n}{d}\right)^2 D^+ t\right]\sin\left(\frac{\pi n x_0}{d}\right)}{\left(\frac{\mu^+ E\,d}{2\pi D^+}\right)^2 + n^2}\right\}. \qquad (8)$$

But even simplifications do not allow the system of equations (8) to be obtained in the analytical form because of the difficulties faced at the summation of the corresponding infinite series. However, the detailed analysis of relations (8) makes it possible to find the analytical functions, to which they best correspond. In turn, this allows one to propose simple analytical dependences for their approximation:

$$E(t) = \left[1 + \exp\left(\frac{\mu^- E\,t - x_0}{\sqrt{\frac{1}{2}\,D^-\,t}}\right)\right]^{-1},$$

$$P(t) = \left[1 + \exp\left(\frac{\mu^+ E\,t - (d - x_0)}{\sqrt{\frac{1}{2}\,D^+\,t}}\right)\right]^{-1}. \qquad (9)$$

The use of approximating relations in the forms of expressions (9) allows, first, the calculations to be made considerably simplified by avoiding the evaluation of the sums of infinite series in Eqs. (8) and, second, allows the current pulse function, which preserves its dependence on the main kinetic parameters of the charge carrier motion, to be described analytically.

The results of calculations of the function $E(t)$ and its approximations by relation (9) made for various values of the charge carrier generation coordinate and the electric field strength are depicted in Figs. 5 and 6 for Si and ZnSe crystals, respectively. It should be noted that, depending on the choice of a semiconductor detector material, the influence on its spectrometric characteristics is mainly determined by three factors: the material purity, efficiency of ionizing radiation registration, and mobility of free charge carriers. Wide-band-gap semiconductors have been considered lately as rather promising in this respect. The same purity degree as for, e.g., silicon, has not been reached for them yet. However, they are characterized by extremely small dark currents (at a level of 1 pA for ZnSe single crystals at a temperature of 300 K and an electric field strength of 500 V/cm) and a high efficiency of ionizing radiation absorption.

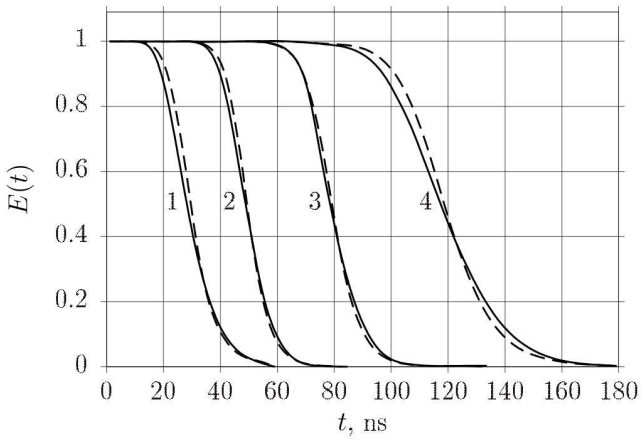

Fig. 6. The same as in Fig. 5, but for a Si-based detector. The curve notation is the same. Calculation parameters are $d = 250$ μm and $\mu^- = 1400$ cm^2/(V × s)

6. Conclusions

A basic model for the kinetics of X-ray conductivity in semiconductors has been proposed. It allows the current pulse shape at the absorption of an X-ray quantum in an ideal semiconductor to be obtained in the first approximation, and the influence of key material parameters and the electric field on the pulse shape to be analyzed. An analytical relation for the current pulse, which arises in the external electric circuit at the absorption of an X-ray quantum, has been proposed, which considerably simplifies the subsequent development of a kinetic model of X-ray conductivity in semiconductors. The next step should consist in determining the influence of the Coulomb interaction between generated free charge carriers and point defects (traps and recombination centers), which always exist in real substances, on the amplitude and the shape of a current pulse that arises at the absorption of an X-ray quantum.

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БАЗОВА КІНЕТИЧНА
МОДЕЛЬ РЕНТГЕНОПРОВІДНОСТІ
ШИРОКОЗОННИХ НАПІВПРОВІДНИКІВ

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Р е з ю м е

При реєстрації рентгенівського кванта напівпровідниковим детектором відбувається генерація вільних носіїв заряду в не-

великому об'ємі (діаметр $< 0{,}5$ мкм). Якщо до електродів напівпровідника прикласти різницю потенціалів, то відбувається направлений рух згенерованих вільних носіїв та відповідний імпульс струму в зовнішньому колі. Запропоновано логічну схему побудови базової кінетичної моделі рентгенопровідності напівпровідників, яка застосовує послідовний у часі розрахунок просторових розподілів вільних носіїв заряду та використовує дифузійно-дрейфову модель руху вільних носіїв у твердому тілі. Отримано базову форму імпульсу струму у зовнішньому колі в аналітичному вигляді для випадку ідеального напівпровідника, тобто такого, що не містить глибоких пасток і центрів рекомбінації. Одержано основні залежності форми імпульсу струму від місця поглинання рентгенівського кванта та величини прикладеного електричного поля.