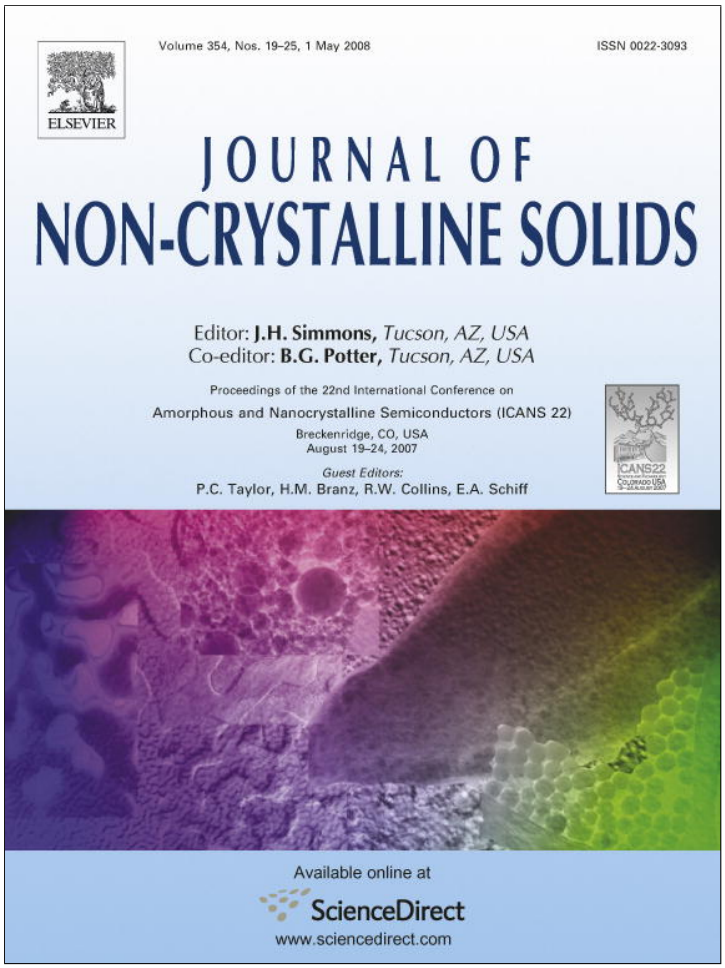

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Scattering and movement asymmetry in the one-dimensional lucky-drift simulation of the avalanche processes in disordered semiconductors

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Abstract

A lucky-drift model for impact ionization has been recently successfully used to account for avalanche phenomenon in amorphous selenium (a-Se). The model presumed angle symmetry for scattering of charge carriers on disorder potential. We check this model by computer simulations in one-dimensional case and show that the analytical formulation used so far essentially underestimates the ionization rate. Furthermore, the scattering symmetry should lead to the dependence of the impact ionization coefficient on the sample thickness. Such dependence has not been experimentally confirmed in a-Se. Therefore, we modify the model taking into account the scattering and movement asymmetry of charge carriers in the applied electric filed. It is shown that in such formulation the impact ionization rate does not depend on the sample thickness in agreement with experimental data.

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Keyword: Amorphous semiconductors

1. Introduction

The process of avalanche multiplication of charge carriers in amorphous semiconductors, particularly in amorphous selenium (a-Se), known since many years [1–5] has received recently a significant attention of the scientific community due to the application of these materials in X-ray imaging devices [6–8] and in harpicon tubes – ultra-high sensitive TV pickup tubes that use avalanche multiplication in a-Se to capture images at extremely low light intensities [9–11]. It has been well established experimentally [5,6] that the avalanche phenomenon is observed in a-Se at electric fields above 0.7 MV/cm.

One possible approach to account for the effect is to apply to a-Se theoretical models initially proposed for crystalline semiconductors, for instance the Shockley lucky-ballistic model [12,13] or the Ridley lucky-drift (LD) model [9,14]. Another approach is to try to modify theoretical models developed for crystalline semiconductors taking into account specific features of amorphous materials. The latter attempt has been recently performed by Rubel et al. [15], who extended for amorphous semiconductors the LD model of Ridley taking into account elastic scattering on disorder potential inherent for amorphous materials. This scattering mechanism has not been included into the models for crystalline semiconductors.

According to the LD model of Rubel et al. [15], charge carrier experiences elastic scattering on disorder potential and inelastic scattering on optical phonons while being accelerated by electric field. The particular formulation of

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this model sounds as follows. (i) The only elastic scattering process is scattering on disorderer potential; the mean free path for the elastic scattering is a model parameter λ; (ii) the loss of energy by a charge carrier in each collision with phonons is constant and equals to the optical phonon energy E_{ph}; the mean free path for the inelastic scattering is another model parameter λ_E; (iii) the collisions with phonons do not change the carrier trajectory essentially. An arbitrary path of a primary charge carrier during its drift as a series of k elastic collisions and m inelastic ones is considered. Further, the elastic collisions are divided into two subcategories: k_l 'lucky' collisions and k_u 'unlucky' ones. After a lucky elastic collision, the velocity of a carrier has a positive projection on the field direction and hence the carrier gains energy from the electric field after the scattering event. In the opposite case, a carrier loses its energy traveling against the field.

The resulting impact ionization coefficient is calculated as

$$\beta = \sum_{m=0}^{\infty} \sum_{k_u=0}^{\infty} \frac{P(k_u, m)}{l(k)}, \tag{1}$$

where the length $l(k)$ of the path for a charge carrier along the field direction after performing $k = k_l + k_u$ elastic collisions in order to attain the energy

$$E_I = k_l eF\lambda\langle\cos\Theta\rangle - k_u eF\lambda\langle\cos\Theta^*\rangle - m\hbar\omega \tag{2}$$

necessary for impact ionization, i.e., to create a secondary charge carrier, was estimated [15] as

$$l(k) = \lambda(k_l\langle\cos\Theta\rangle + k_u\langle\cos\Theta^*\rangle). \tag{3}$$

$\langle\cos\Theta\rangle$ and $\langle\cos\Theta^*\rangle$ are the projections of the carrier velocity on the direction of electric field averaged over lucky and unlucky scattering events, respectively. The probability for charge carrier to experience the favorable for impact ionization chain of events

$$P(k_u, m) = P_{el}(k_u)P_{il}(k, m) \tag{4}$$

is a product of the probability P_{el} to have k_u unlucky collisions in the chain of k elastic scattering events

$$P_{el}(k_u) = \frac{[k(1-W)]^{k_u}}{k_u!}\exp[-k(1-W)] \tag{5}$$

and the probability P_{il} to have m inelastic collisions in the same chain

$$P_{il}(k, m) = \frac{(k\lambda/\lambda_E)^m}{m!}\exp[-k\lambda/\lambda_E]. \tag{6}$$

In Eq. (5), W is the probability for a carrier to be reflected within the angle $\Theta \leqslant \pi/2$.

The crucial assumptions made in the initial calculations in the framework of this model [15] were the assumption on the angular symmetry of the elastic scattering collisions and also the assumption that external electric field supplies charge carriers with energy after lucky collisions though it does not affect the direction of the velocity after the collision event. Concomitantly W was assumed in [15] equal to 1/2.

The purpose of this paper is to check the validity of this approach by straightforward computer simulations. We perform a Monte Carlo simulation of the avalanche phenomenon in the LD model as formulated by Rubel et al. [15]. A one-dimensional system is considered as a test field. The results of the simulation show that Eqs. (1)–(6) underestimate the ionization rate. Moreover, the simulation results predict the ionization rate in the symmetrical formulation of the LD model to be dependent on the thickness of the sample under study. Experimental results in a-Se however do not indicate such a dependence on the sample thickness [3,5]. Therefore, it is necessary to improve the LD model. We perform such an improvement taking into account both the asymmetry of the elastic scattering and that of the carrier motion caused by electric field. The results of the improved theory appear independent of the sample thickness in accord with experimental results. In Section 2 we briefly describe the simulation algorithm. In Section 3 we present the simulation results for the symmetrical formulation of the LD model. In Section 4 the improved LD model is formulated taking the asymmetry effects into account and the simulation results obtained within this model are presented. Concluding remarks are given in Section 5.

2. The model

For simplicity we consider a one-dimensional chain of sites along the external electric field F. A charge carrier (hole in our case) drifts in this chain suffering momentum-relaxing scattering from random potential fluctuations after each λ traversed distance. For each scattering event there are two choices for the carrier: to propagate along the field F and hence to gain the energy $eF\lambda$ or to travel against the field and hence to lose the energy $eF\lambda$. In simulation process one can introduce corresponding P_l and P_u probabilities, divide $x = [0;1]$ numerical segment in two subsegments $x_l = [0; P_l/(P_l + P_u)]$ and $x_u = [P_l/(P_l + P_u); 1]$, generate a random number and check: if generated number falls into x_l subsegment then a carrier propagates along the field and in the opposite case – travels against the field direction. In addition to the elastic scattering from random potential fluctuations, the inelastic scattering by optical phonons with corresponding probability determined by another simulation parameter $\lambda_E > \lambda$ is also taken into account. Again one can introduce corresponding $x_{ph} = [0; \lambda/\lambda_E]$ numerical subsegment, generate another random number and if this number falls into subsegment x_{ph}, then a carrier suffers an energy-relaxing scattering and loses energy $E_{ph} = \hbar\omega$. In the spirit of Ref. [15] we assume that the inelastic scattering changes carrier's energy, but not its trajectory. Ionization energy E_I is gained as a result of the lucky-drift with a sequence of elastic and inelastic collision events. We consider an abrupt process assuming that impact ionization occurs immediately once

the threshold energy is reached and hence the primary charge carrier is at zero energy just after the ionization event. The process described above should be continued until the whole distance traveled by a charge carrier attains the sample thickness d. Then the impact ionization coefficient can be calculated by counting the number of ionization events N as

$$\beta = \frac{N}{d}. \tag{7}$$

The set of simulation parameters includes: threshold ionization energy E_I, optical phonon energy E_{ph}, elastic scattering mean free path λ, inelastic scattering mean free path λ_E and electric field F. The first two parameters are usually known: in a-Se, $E_{ph} = 0.031$ eV [3,16–18] and $E_I = 2.3$ eV (E_I is assumed to be equal to the width of the mobility gap since for a-Se the ionizing excitation across the mobility gap is more probable than the excitation from localized states within the mobility gap [2]). Therefore, λ and λ_E remain only actual simulation parameters for the given field.

3. Simulation results with the scattering and movement symmetry

The aim of this section is to verify the analytical expression for the impact ionization coefficient obtained in Ref. [15] by performing a direct computer simulation of the avalanche in a one-dimensional chain of collision events. The LD model presumes the scattering processes to be spherically symmetrical [15]. In terms of our simulation this means that $P_l = P_u$ for each collision event.

In the test simulation we select the sample thickens of 20 μm, which is in the experimentally-relevant range of 5–50 μm. The model parameters are close to those used previously to describe impact ionization in a-Se [20] ($E_I = 2.3$ eV, $\lambda = 3$ Å, $\lambda_E = 24$ Å, $E_{ph} = 0.031$ eV). As a result of computer simulation we obtain the impact ionization coefficient $\beta = 640 \pm 600\ \mathrm{cm}^{-1}$ averaged over 50 independent realizations. The corresponding analytical value of the impact ionization coefficient calculated from Eq. (1) is $\beta = 1.7 \times 10^{-10}\ \mathrm{cm}^{-1}$, which is by 12 order of magnitude less than the corresponding simulation result. This indicates that the analytical expression significantly underestimates the number of ionization events.

Furthermore, we check by computer simulation the dependence of the ionization coefficient on the sample thickness. Results are shown in Fig. 1 for the sample thicknesses in the range $d = 20$–100 μm. It is evident from Fig. 1, that the ionization coefficient increases with increasing of the sample thickness. This result contradicts to the experimental observations indicating thickness independence of the ionization coefficient, at least for the range of $d = 5$–50 μm [3,5,20].

The dependence of the ionization coefficient on the sample thickness found in the computer simulation is due to the diffusive character of the carrier movement. The carrier trajectory length is not equivalent to the sample thickness,

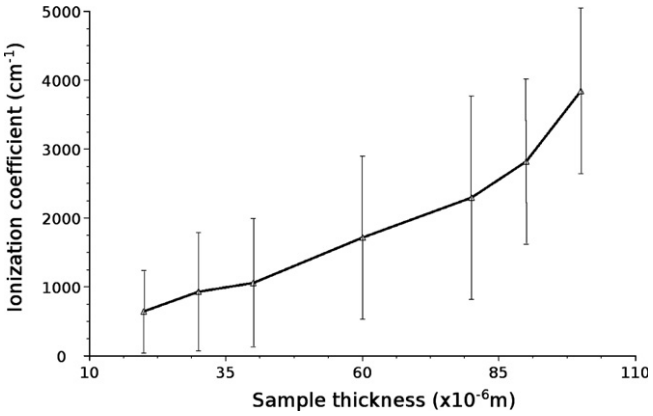

Fig. 1. Impact ionization coefficient vs sample thickness in the case of scattering and movement symmetry. a-Se, $E_I = 2.3$ eV, $\lambda = 3$ Å, $\lambda_E = 24$ Å, $E_{ph} = 0.031$ eV, $F = 1.0$ MV/cm.

and it increases nonlinearly (as n^2) with the number of scattering events n. Therefore, the number of ionization events depends superlinearly on the sample thickness. Concomitantly, the impact ionization coefficient determined as the ratio between the number of ionization events and the sample thickness turns out to be dependent on the thickness.

In order to overcome this deficiency we modify below the described approach taking into account asymmetry effects for carrier scattering by disorder potential and carrier movement with respect to the field direction.

4. Simulation results with the scattering and movement asymmetry

There are two kinds of asymmetry that are to be taken into account. First – the scattering asymmetry with respect to the carrier velocity. For simplicity we consider elastic scattering as scattering on potential well $U = -U_0$ for $r < a$ and $U = 0$ for $r > a$, where U_0 is the energetic depth and a – the width of the well. (We choose the values $U_0 \approx 0.0125$ eV and $a \approx 3$ Å for a-Se). In the Born approximation the corresponding scattering differential cross-section can be estimated as [19]

$$\frac{d\sigma}{d\Omega} = \sigma_0 \exp\left[-\frac{E}{E_0}\sin^2\frac{\varphi}{2}\right], \tag{8}$$

where

$$\sigma_0 = \frac{\pi a^2}{4}\left[\frac{m^* U_0 a^2}{\hbar^2}\right]^2, \quad E_0 = \frac{\hbar^2}{4m^* a^2}, \tag{9}$$

φ is the scattering angle, m^* – the carrier effective mass.

Using Eqs. (8) and (9) one can estimate the probabilities for a carrier to be scattered within the angle $\varphi \leqslant \pi/2$, $P_{\varphi\leqslant\pi/2} = \int_0^{\frac{\pi}{2}} (d\sigma/d\Omega)\sin\varphi\, d\varphi$ and within the angle $\varphi > \pi/2$, $P_{\varphi>\pi/2} = \int_{\frac{\pi}{2}}^{\pi} (d\sigma/d\Omega)\sin\varphi\, d\varphi$. Then the ratio of P_l and P_u probabilities is equal to

$$\alpha_s^d(E) \equiv \frac{P_l}{P_u} = \frac{1-\exp(-\frac{E}{2E_0})}{\exp\left(-\frac{E}{2E_0}\right)-\exp\left(-\frac{E}{E_0}\right)} \tag{10}$$

for a carrier moving along the field before the collision and

$$\alpha_s^a(E) = \left[\alpha_s^d(E)\right]^{-1} \tag{11}$$

in the opposite case.

Another kind of asymmetry is the movement asymmetry with respect to the direction of the electric field. For a given initial energy the probability for a carrier to propagate along the field, Q_l is higher then that to travel against the field, Q_u. We assume that these probabilities can be determined as a reciprocal times, spent by a carrier during its motion from one scattering center to the next one. Then the motion asymmetry determined as a ratio of Q_l and Q_u is described by

$$\alpha_m(E) \equiv \frac{Q_l}{Q_u} = \left(\sqrt{1+\frac{eF\lambda}{E}}-1\right)\left(1-\sqrt{1-\frac{eF\lambda}{E}}\right)^{-1} \tag{12}$$

Eq. (12) is valid only if $E > eF\lambda$. Indeed, if the initial energy E is not enough to overcame the energy loss at distance λ travelled against the field between two neighboring centers, then the carrier will simply turn back without any scattering event and continue its motion along the field. In our simulation it means that $P_l = 1$, $Q_l = 1$ and consequently, $P_u = 0$, $Q_u = 0$.

The energy dependences $\alpha_s^d(E), \alpha_s^a(E)$ and $\alpha_m(E)$ are shown in Fig. 2 for $\lambda = 3$ Å and $F = 1.0$ MV/cm. One can see that the scattering asymmetry is important for high energies and the movement asymmetry – for low ones: the scattering for low energies is almost isotropic and the influence of the field is significant at low carrier velocity.

The simulation algorithm for the case of the scattering and movement asymmetries is more complicated than in the symmetrical case. For each elastic scattering event one should introduce two (instead of one in the symmetrical case) numerical segments: $X^s = [0;1]$ and $X^m = [0;1]$,

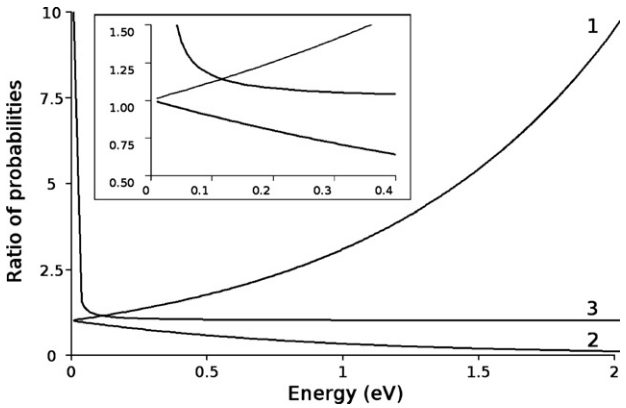

Fig. 2. (1) Scattering asymmetry for a carrier moving along the field before the collision (α_s^d), (2) scattering asymmetry for a carrier moving against the field before the collision (α_s^a) and (3) movement asymmetry (α_m).

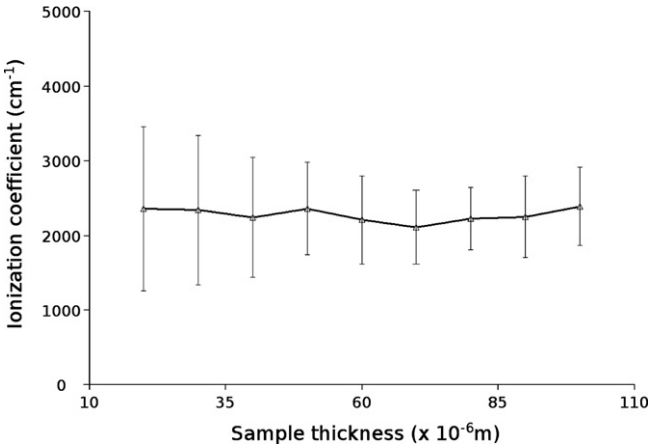

Fig. 3. Impact ionization coefficient vs sample thickness in the case of the scattering and movement asymmetries. a-Se, $E_I = 2.3$ eV, $\lambda = 3$ Å, $\lambda_E = 24$ Å, $F = 1.0$ MV/cm.

divide X^s into two subsegments $X_l^s = [0;\alpha_s/(1+\alpha_s)]$ and $X_u^s = [\alpha_s/(1+\alpha_s);1]$ ($\alpha_s = \alpha_s^d$ or $\alpha_s = \alpha_s^a$ depending on the movement direction of the carrier before the collision) and X^m – into subsegments $X_l^m = [0;\alpha_m/(1+\alpha_m)]$ and $X_u^m = [\alpha_m/(1+\alpha_m);1]$, generate two random numbers n_1 and n_2 and check: if n_1 falls into X_l^s and n_2 falls into X_l^m then a carrier propagates along the field. If n_1 falls into X_u^s and n_2 falls into X_u^m then a carrier moves against the field. The situation becomes more complicated if n_1 falls into X_l^s and n_2 falls into X_u^m or n_1 falls into X_u^s and n_2 falls into X_l^m. Then the additional subsegments $X_1^{ad} = [0;P_l/(P_l+Q_u)]$ and $X_2^{ad} = [P_l/(P_l+Q_u);1]$ are needed for the former case and $X_1^{ad} = [0;Q_l/(Q_l+P_u)]$ and $X_2^{ad} = [Q_l/(Q_l+P_u);1]$ for the latter one, and the additional random number n_3 should be generated. If n_3 falls into X_1^{ad} then a carrier propagates along the field. In the opposite case – against the field.

The results of our simulation for the same parameters as used in the symmetrical case: $\lambda = 3$ Å, $\lambda_E = 24$ Å, $F = 1.0$ MV/cm and various sample thicknesses are shown in Fig. 3. It is clear that the impact ionization coefficient does not (at least within the simulation accuracy shown as the error bars) depend on the sample thickness. This is the main result of our improved consideration.

5. Conclusions

The lucky-drift model suggested previously for description of the impact ionization in amorphous semiconductors is extended taking into account the angular asymmetry in scattering of charge carrier by disorder potential and the effect of the electric field on the asymmetry in the carrier movement. Only a one-dimensional case is studied. The results of Monte Carlo computer simulations show that the model in its previous version with the symmetrical angular scattering and the symmetrical charge movement with respect to the field direction essentially underestimates the impact ionization coefficient. Furthermore, it is shown that the symmetrical model yields the ionization coefficient

dependent on the sample thickness. This result is not confirmed by experimental data. The modified model yields the ionization rates, which appear independent of the sample thickness.

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