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A lucky-drift (LD) model for impact ionization has been recently successfully used to account for avalanche phenomenon in amorphous semiconductors. This model however leads to the dependence of the impact ionization coefficient on the sample thickness. However such dependence has not been confirmed experimentally. Recently LD model has been improved taking into account the scattering and movement asymmetry of charge carriers in the applied electric field. As a result, the impact ionization coefficient was obtained independent on the sample thickness. We apply the improved LD model to study the field dependence of the impact ionization coefficient in a-Se, a-Si:H and Ge2Sb2Te5. We show that even in one-dimensional formulation of the improved LD model the agreement between theoretical results and experimental data evidenced in a-Se is better than that in the formulation with scattering and movement symmetry.

1 Introduction Avalanche multiplication in amorphous semiconductors is used in X-ray imaging devices to obtain detectors with high sensitivity at low exposures [1, 2], in harpicon tubes – ultrahigh sensitive TV pickup tubes to capture images at extremely low light intensities [3, 4], and in memory-storage devices for transition of the phase-change material between amorphous and crystalline phase [5]. So far amorphous selenium (a-Se) is mainly used for the two former purposes and alloy material $Ge_2Sb_2Te_5$ (GST) - for the latter one.

Avalanche multiplication of photogenerated holes in a-Se was first reported by Juska et al. [6, 7] and later by Tanioka and co-workers [8, 9] at very high fields (80 MV/m). To the best of our knowledge, a-Se is still the only amorphous semiconductor that clearly evidences reproducible avalanche multiplication. Although, recently Pirovano et al. [5] have suggested that impact ionization is a precursor for the switching effect in GTS, there is still no direct experimental evidence of the avalanche multiplication in this material. Another prototype amorphous semiconductor is hydrogenated amorphous silicon (a-Si:H). Attempts to reach avalanche multiplication for electric fields below 80 MV/m have been futile [10, 11] even though the bandgap of a-Si:H (1.7 – 1.8 eV) is smaller than that for a-Se (2.0 – 2.3 eV). However, Akiyama et al. [12] reported avalanche multiplication within a i-type a-Si:H at higher fields (about 150 MV/m),

One possible approach to account for the effect is to apply to the amorphous semiconductors theoretical models initially proposed for crystalline semiconductors, for instance the Shockley lucky-ballistic model [13] or the Ridley lucky-drift (LD) model [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 carriers experience elastic scattering on disorder potential and inelastic scattering on optical phonons while being accelerated by electric field. The resulting impact ionization coefficient is calculated as a ratio of the probability for charge carrier to experience the favourable for impact ionization chain of scattering events and the length of the path for a charge carrier along the field direction in the same chain.

In Ref. [16] this LD approach was applied to study the impact ionization in a-Se, a-Si:H and in a-GTS. As it was mentioned above, the only material where the avalanche multiplication phenomenon have been clearly evidenced, is a-Se. So, the elastic scattering mean free path λ and inelastic scattering mean free path λ_E of the carrier were chosen from the best fit to the observed field dependence of the impact ionization coefficient in this material [17]. It was shown that for the similar values of λ and λ_E the LD model is capable to account for the magnitude of the electric fields necessary to launch the avalanche phenomenon not only in a-Se, but also in a-Si:H and in a-GST. Furthermore, the results suggest that the higher phonon energy in a-Si:H and the lower one in a-GST as compared to a-Se, shift the threshold field for impact ionization in a-Si:H to essentially higher and in a-GST – to essentially lower fields than those needed for avalanche multiplication in a-Se.

Two crucial assumptions were made in the model formulated in Ref. [15]: (i) the angular symmetry of the elastic scattering collisions and (ii) the assumption that external electric field does not affect the direction of the velocity after the collision event. In Ref. [18] the validity of this approach was checked by straightforward Monte Carlo simulation of the impact ionization in a-Se. The results of the simulation showed that LD model with the scattering and movement symmetry underestimate the ionization rate. Moreover, the simulation results predict the ionization rate 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 [7]. The LD model have been improved [18] 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 the experimental observation [7].

The purpose of this paper is to apply the improved LD model to study the field dependences of the impact ionization coefficient in a-Se, a-Si:H and a-GST. In Sec.2 we briefly describe the model and the simulation algorithm. In Sec. 3 the simulation results are presented. Concluding remarks are given in Sec. 4.

2 The model and the simulation algorithm For simplicity we consider a one-dimensional chain of sites along the external electric field F. A charge carrier drifts in this chain experiencing momentum-relaxing scattering from random potential fluctuations after each λ traversed distance and the inelastic scattering by optical phonons after each λ_E traversed distance. For each elastic 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 the improved asymmetrical LD model (in contrary to the previous symmetrical one) the corresponding probabilities are not equal. There are two kinds of asymmetry that are to be taken into account: (i) the scattering asymmetry with respect to the carrier velocity and (ii) the movement asymmetry with respect to the direction of the electric field.

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 $U_0 = 0.0125\,\text{eV}$ and assume that $a = \lambda$). The scattering asymmetry is caused by the dependence of the scattering differential cross-section on the scattering angle φ and the carrier energy E. In the Born approximation this dependence can be estimated as [19]:

$$\frac{d\sigma}{d\Omega} = \sigma_0 \exp\left[-\frac{E}{E_0}\sin^2\frac{\varphi}{2}\right], \tag{1}$$

where

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

m^* - the carrier effective mass.

Using Eqs. (1), (2) one can estimate the probabilities for a carrier to be scattered within the angle $\varphi \le \pi/2$,

$$P_{\varphi\le\pi/2} = \int_0^{\pi/2} (d\sigma/d\Omega)\sin\varphi \;\; d\varphi, \tag{3}$$

and within the angle $\varphi > \pi/2$,

$$P_{\varphi>\pi/2} = \int_{\pi/2}^{\pi} (d\sigma/d\Omega)\sin\varphi \;\; d\varphi. \tag{4}$$

Then the ratio of the probabilities for a charge carrier with the energy E to be scattered along the filed P_l and against the filed P_u is equal to:

$$\alpha_s^d(E) \equiv \frac{P_l}{P_u} = \frac{1-\exp\left(-\dfrac{E}{2E_0}\right)}{\exp\left(-\dfrac{E}{2E_0}\right)-\exp\left(-\dfrac{E}{E_0}\right)} \tag{5}$$

for a carrier moving along the field before the collision and

$$\alpha_s^a(E) = \left[\alpha_s^d(E)\right]^{-1} \tag{6}$$

in the opposite case.

The movement asymmetry is determined as a ratio of the probability for a carrier to propagate along the field, Q_l, and that to travel against the field, Q_u (of course $Q_l > Q_u$

for a given initial energy). We assume that these probabilities can be determined as a reciprocal times spent by a carrier during its motion from one scattering centre to the next one. Then the motion asymmetry is described by

$$\alpha_m(E) \equiv \frac{Q_l}{Q_u} = \frac{\sqrt{1+\dfrac{eF\lambda}{E}}-1}{1-\sqrt{1-\dfrac{eF\lambda}{E}}} \quad . \tag{7}$$

Eq.(7) is valid only if $E > eF\lambda$. Indeed, if the initial energy E is not enough to overcome the energy loss at distance λ travelled against the field between two neighbouring centres, the carrier will 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, $P_u = 0$, $Q_u = 0$. From Eqs. (5)-(7) one can see that the scattering asymmetry is significant for high energies and the movement asymmetry for low ones.

The simulation algorithm is the following. For each scattering event one should introduce two numerical segments: $X^s = [0;1]$ and $X^m = [0;1]$, divide X^s into two subsegments $X_l^s = [0;\alpha_s/(1+\alpha_s)]$ and $X_m^s = [\alpha_s/(1+\alpha_s);1]$ ($\alpha_s = \alpha_s^d$ 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 $X_l^m = [\alpha_m/(1+\alpha_m);1]$. One should 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 if n_1 falls into X_u^s and n_2 falls into X_l^m. Then the additional subsegments $X_1^{ad} = [0;P_l/(P_l+Q_m)]$ and $X_2^{ad} = [P_l/(P_l+Q_m);1]$ are needed for the former case and $X_1^{ad} = [0;Q_l/(P_u+Q_l)]$ and $X_2^{ad} = [Q_l/(P_u+Q_l);1]$ for the later 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. Besides, the additional numerical segment $X^{ph} = [0;1]$ and the additional random number n_4 are needed to take into account the inelastic scattering by optical phonons. If n_4 falls into subsegment $X_u^{ph} = [0;\lambda/\lambda_E]$ then a carrier experiences an energy-relaxation 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 travelled 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

$$\beta = \frac{N}{d} \tag{8}$$

The set of simulation parameters includes: threshold ionization energy E_I, optical phonon energy E_{ph}, the elastic scattering mean free path λ, and the inelastic scattering mean free path λ_E. The first two parameters are usually known. Therefore only λ and λ_E remain actual simulation parameters for the given field.

3 Simulation results for a-Se, a-Si:H and a-GST

In order to calculate the impact ionization coefficient we need to specify material parameters. As it was mentioned in the previous section, E_I and E_{ph} are usually known. Their values for a-Se, a-Si:H and a-GST are given in Table 1.

Table 1 Ionization energy and optical phonon energy in a-Se, a-Si:H and a-GST.

Material	Ionization energy (eV)	Optical phonon energy (eV)
a-Se [7, 20]	2.3	0.031
a-Si:H [21, 22]	1.8	0.08
a-GST [5, 23]	0.7	0.02

E_I is assumed to be equal to the width of the mobility gap [5, 6]. The values of λ and λ_E used in our simulation are collected in Table 2 together with those used in previous consideration with scattering and movement symmetry [16].

Table 2 Elastic scattering mean free path λ and inelastic scattering mean free path λ_E in a-Se, a-Si:H and a-GST.

Material	LD with scattering and movement symmetry [16]		LD with scattering and movement asymmetry	
	λ (Å)	λ_E (Å)	λ (Å)	λ_E (Å)
a-Se	6	72	3	24
a-Si:H	6	72	3	24
a-GST	10	70	3	120

In the spirit of Ref. [16], λ and λ_E are considered to be free parameters and are chosen from the best fit to the field dependences of the multiplication coefficient evidenced in a-Se [17]. The same values are used for a-Si:H though for a-GST the value of λ_E being essentially higher with the aim to account for the magnitude of the electric fields necessary to launch the avalanche phenomenon in this material. It should be mentioned that the values of λ in our simulation with scattering and movement asymmetry are essentially lower than those suggested by previous consideration with scattering and movement symmetry. The values of λ became closer to the interatomic distance, i.e., the length scale of disordered potential.

The field dependences of the impact ionization coefficient in a-Se, a-Si:H and a-GST averaged over 50 independent realizations of our Monte Carlo simulation are shown in Fig. 1. (For the comparison purpose the field dependences of the ionization coefficient obtained by means of the LD model with scattering and movement symmetry [16] as well as the experimental results for a-Se [17] are also shown in this figure.)

One can see that the agreement between the theoretical results obtained by improved LD model and the experimental data for a-Se is somewhat better than that obtained by previous LD model. The agreement however is not still satisfactory. The reason might be the simplified (one-dimensional) treatments of the model. We hope that two- and three-dimensional simulation of the impact ionization phenomenon in amorphous semiconductors would lead to further improvements in the agreement between theoretical results and experimental data.

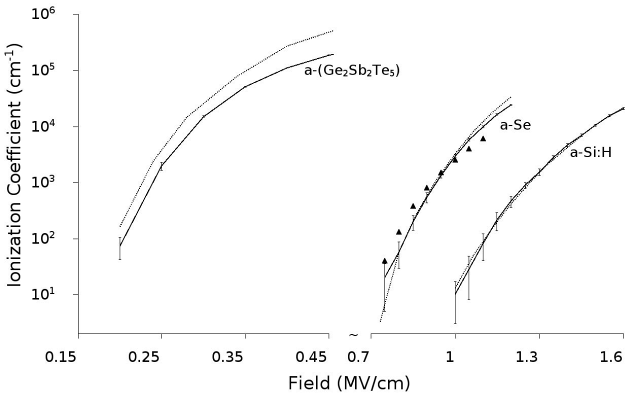

Figure 1 Ionization coefficient vs. electric field in a-Se, a-Si:H and a-GST; solid curves – results of the LD model with scattering and movement asymmetries, dotted curves – results of the LD model with scattering and movement symmetries [16], triangles – experimental result for a-Se [17].

4 Conclusions The lucky-drift model suggested previously for description of the impact ionization in amorphous semiconductors assumes the symmetrical angular scattering and the symmetrical charge movement with respect to the field direction. This model was applied to study the field dependence of the impact ionization coefficient in a-Se, a-Si:H and a-$Ge_2Sb_2Te_5$ [16]. It was shown that for certain values of the elastic scattering mean free path λ, and the inelastic scattering mean free path λ_E LD model is capable to account for the magnitude of the electric fields necessary to launch the avalanche phenomenon in these materials.

We perform Monte Carlo simulation of the impact ionization processes in amorphous materials on the basis of the improved LD model 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. A one-dimensional case is studied. The results of Monte Carlo simulations show that the values of λ in the improved LD model are closer to the interatomic distance, i.e. to the length scale of disordered potential in the materials under consideration than in the symmetrical case. The agreement between theoretical results obtained by the improved LD model with scattering and movement asymmetry and experimental data evidenced for a-Se is better than that obtained by previous LD model with scattering and movement symmetry.

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