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CONTRIBUTION OF INTERNAL IONIZATION PROCESSES IN SEMICONDUCTORS TO RADIATIVE LOSSES OF RELATIVISTIC ELECTRONS

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The study presents analysis of mass radiative energy losses (RL) incurred by relativistic electrons in different materials commonly used in semiconductor electronics. We have specifically focused on accounting for the processes of 'internal' ionization, resulting in the production of electron-hole pairs in semiconductors and dielectrics. We have established that accounting for these processes is the only method offering consistent explanations on the values of mass RLs observed experimentally. The analysis performed should allow to make more detailed predictions for the performance of semiconductor devices in real conditions, particularly, in space.

Keywords: relativistic electron, ionization potential, radiative energy losses, silicon, germanium, graphene

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ВКЛАД ПРОЦЕССОВ ВНУТРЕННЕЙ ИОНИЗАЦИИ ПОЛУПРОВОДНИКОВ В ТОРМОЗНЫЕ ПОТЕРИ ЭНЕРГИИ РЕЛЯТИВИСТСКИХ ЭЛЕКТРОНОВ

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Выполнен анализ массовых тормозных потерь энергии (ТПЭ) релятивистских электронов в различных материалах, используемых в полупроводниковой электронике. Особое внимание уделено учету процессов «внутренней» ионизации, приводящей к образованию электронно-дырочных пар в полупроводниках и диэлектриках. Показано, что только при таком учете удается непротиворечиво объяснить экспериментально наблюдаемые значения массовых ТПЭ. Проведенный в работе анализ позволит выполнять более детальное прогнозирование работоспособности полупроводниковых приборов в реальных, в частности космических, условиях.

Ключевые слова: релятивистский электрон, потенциал ионизации, тормозные потери энергии, кремний, германий, графен

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Introduction

While the effects of electron irradiation on the properties of semiconductor structures and devices have been considered in numerous papers and books [1 – 4], many aspects of this problem are yet to be fully understood. Most studies tend to focus on the role of elastic processes and the effect of emerging radiation defects on the properties of materials and devices [4 – 8]. The contribution from inelastic energy losses of bombarding particles is discussed to a far lesser extent. However, it is the inelastic processes that determine the resistance to electron radiation for a number of semiconductor devices, e.g., metal-oxide-semiconductor (MOS) structures and field-effect transistors [9].

The goal of our study is to investigate the ionization losses and the absorbed energy of relativistic electrons in different materials used in semiconductor electronics. In particular, we concentrated on the processes of 'internal' ionization leading to production of electron-hole pairs in semiconductors and dielectrics. Relativistic electrons of 0.9 MeV ($V = 0.94c$) were used as irradiating particles. The particles and the energy were chosen so that the computational data could be verified experimentally with the RTE-1V electron accelerator available at Peter the Great St. Petersburg Polytechnic University.

Estimation of radiative energy losses of relativistic electrons within the Born approximation of scattering theory

In general, calculating the absorbed energy is a complex problem that can be best solved by numerical methods. We confine ourselves to considering the situation when the thickness of the irradiated sample is much lower than the particle range, which is the case in most applied problems.

The absorbed dose D_e depends on linear radiative losses (RL) of the bombarding electrons (dE/dx) in the medium:

$$D_e = (1/\rho)\cdot(dE/dx)F_e. \qquad (1)$$

Here ρ is the density of the medium, F_e is the exposure dose, often referred to as fluence.

The quantity $(1/\rho)\cdot(dE/dx)$ which is called the reduced (or mass) RL, is more common in practice. For convenience, Eq. (1) can be transformed by introducing the units widely used for the quantities included in this formula:

$$D_e = 1.6\cdot 10^{-10}(1/\rho)\cdot(dE/dx)F_e; \qquad (2)$$

D_e is given here in grays (Gy), mass RL $(1/\rho)\times\times(dE/dx)$ in MeV·(cm²/g), F_e in cm^{-2}.

Eq. (2) allows calculating the absorbed dose at a known particle fluence. The inverse formula for estimation of the fluence required to obtain a known absorbed dose takes the following form:

$$F_e = \frac{1}{1.6\cdot 10^{-10}\left(1/\rho\right)\cdot\left(dE/dx\right)}. \qquad (3)$$

The stopping power of MeV electrons is mainly due to ionization and excitation of bound electrons in target atoms (ionizing losses). Therefore, the notions of radiative and ionizing energy losses are virtually identical in this case. Ionizing energy losses (IEL) of relativistic electrons due to excitation and ionization of target electrons are described by the Bethe formula obtained within the Born approximation of scattering theory [10]:

$$-\left(\frac{dE}{dx}\right)_{ion} = \frac{2pN_{at}Ze^4}{m_eV^2}\times$$
$$\times\left(\ln\frac{m_eV^2E}{2I^2(1-\beta^2)} - \ln 2\left(2(1-\beta^2)^{1/2} - 1 + \beta^2\right) + \right.$$
$$\left. +1-\beta^2+\frac{[1-(1-\beta^2)^{1/2}]^2}{8}\right), \qquad (4)$$

where E is the kinetic energy of the relativistic electron, V is the velocity of the incident electron,

$\beta = V/c$ is the relativistic factor, I is the mean ionization potential of the target atoms.

IEL linearly depend on the number of electrons per unit of the target volume (electron density), N_e. Electron density, in turn, is known to be proportional to the density of the medium:

$$N_e = Z \cdot N_{at} = Z \cdot \rho \cdot N_0 / A. \tag{5}$$

Here N_0 is the Avogadro constant; A is the atomic mass of the medium.

The first (logarithmic) term in curly brackets in the Bethe formula (4) exceeds the remaining terms by an order of magnitude in the given examples. For this reason, Eq. (4) can be simplified by omitting all terms except the first one.

$$-\left(\frac{dE}{dx}\right)_{ion} = \frac{2\pi N_{at} Z e^4}{m_e V^2}\left(\ln\frac{m_e V^2 E}{2\,I^2(1-\beta^2)}\right). \tag{6}$$

Let us express the squared initial velocity of the incident electron in terms of the relativistic factor

$$-\left(\frac{dE}{dx}\right)_{ion} = \frac{2\pi N_{at} Z e^4}{m_e \beta^2 c^2}\left(\ln\frac{m_e \beta^2 c^2 E}{2\,I^2(1-\beta^2)}\right). \tag{7}$$

Let us rewrite the factor in front of the logarithm in expression (7), introducing the Rydberg energy E_{R} and the Bohr radius r_0 widely used in atomic physics:

$$\begin{aligned}-\left(\frac{dE}{dx}\right)_{ion} &= \frac{8\pi N_{at} Z E_{\mathrm{R}}{}^2 r_0{}^2}{m_e \beta^2 c^2}\times \\ &\times\left(\ln\frac{m_e \beta^2 c^2 E}{2I^2(1-\beta^2)}\right),\end{aligned} \tag{8}$$

$$\begin{aligned}E_{\mathrm{R}} &= -\frac{m_e e^4}{2\left(4\pi\varepsilon_0\right)^2 \hbar^2} = 13.6\ \text{eV}, \\ r_0 &= \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2} = 0.53\cdot 10^{-8}\,\text{cm}.\end{aligned} \tag{9}$$

Now Eq. (8) can be used for linear IEL to obtain the formula for mass RL $(1/\rho)\cdot(dE/dx)$, given that the density of the medium $\rho = A \cdot N_{at}/N_0$:

$$\begin{aligned}-\frac{1}{\rho}\left(\frac{dE}{dx}\right)_{ion} &= \frac{8\pi N_{\mathit{ABO\Gamma}} E_{\mathrm{R}}{}^2 r_0{}^2}{m_e c^2}\times \\ &\times\frac{Z}{A\cdot\beta^2}\left(\ln\frac{m_e \beta^2 c^2 E}{2I^2(1-\beta^2)}\right).\end{aligned} \tag{10}$$

Or, substituting the universal constants, we arrive to:

$$\begin{aligned}-\frac{1}{\rho}\left(\frac{dE}{dx}\right)_{ion} &\left(\text{MeV}\cdot\text{cm}^2/\text{g}\right) = \\ &= 0.154\cdot\frac{Z}{A\cdot\beta^2}\left(\ln\frac{0.511\cdot 10^6\cdot\beta^2 E}{2I^2(1-\beta^2)}\right).\end{aligned} \tag{11}$$

It is often assumed that normalized linear IEL reduced to electron density in the target (or normalized mass RL reduced to mass-to-charge ratio of the target nucleus),

$$\begin{aligned}\frac{1}{\rho}\left(\frac{dE}{dx}\right)_{ion}&\left(\frac{A}{Z}\right) = \\ &= \frac{1}{\beta^2}\left(\ln\frac{m_e \beta^2 c^2 E}{2I^2(1-\beta^2)}\right) = K(Z),\end{aligned} \tag{12}$$

is a quantity independent of the material of the stopping target, equal to $18/\beta^2$ [11]. This implies that the contribution from variation of the mean ionization potential under the logarithm in Eq. (11) is small. Making this assumption, we can use Eq. (11) to easily calculate mass RL in any medium based on the experimentally found RL, for example, in aluminum [12]:

$$\begin{aligned}\left(\frac{1}{\rho}\cdot\frac{dE}{dx}\right)_x &= \left(\frac{1}{\rho}\cdot\frac{dE}{dx}\right)_{\mathrm{Al}}\times \\ &\times\left(\frac{Z}{A}\right)_x \Big/ \left(\frac{Z}{A}\right)_{\mathrm{Al}}.\end{aligned} \tag{13}$$

We believe that neglecting the contribution from the ionization potential of the target atoms and using Eq. (13) is ill-suited for our problems. For this reason, Eq. (11) was used to calculate RL in some materials common for semiconductor electronics. Semiconductors with different band gaps, and metals with different ohmic and rectifying contacts were selected. The mean ionization potential I and mass RL of electrons were approximated for these materials. The value of I was taken equal to Ref. [13]:

$$\begin{gathered} I = 11.5Z \text{ (for } Z < 15\text{)}, \\ I = 9.0Z \text{ (for large } Z\text{)}. \end{gathered} \tag{14}$$

The data obtained are given in Table 1. The table also lists the coefficients for calculating the absorbed dose at a known fluence (by Eq. (2)) and calculating the fluence at a known absorbed dose (by Eq. (3)).

As evident from Table 1, mass RL and conversion factors between the exposure and absorbed doses can differ by 1.7 times for most materials (with the atomic number Z ranging from 6 to 79).

The Bragg rule was used for the case when the stopping medium was a chemical compound consisting of several elements [13]. According to this rule, the stopping power of a complex substance is equal to the weighted sum of stopping powers of the constituent elements:

$$\frac{1}{\rho}\cdot\frac{dE}{dx} = \frac{\omega_1}{\rho_1}\cdot\left(\frac{dE}{dx}\right)_1 + \frac{\omega_2}{\rho_2}\cdot\left(\frac{dE}{dx}\right)_2 \tag{15}$$

where ω_1 and ω_2 are the relative proportions of elements in the compound (wt. %).

Eq. (15) was used to calculate the stopping powers of silicon oxide (dielectric) and silicon carbide (wide-bandgap semiconductor). Both values of $1/\rho\cdot(dE/dx)$ coincided and were equal to 1.61 MeV·(cm^2/g).

Fig. 1 shows the curve for mass RL normalized to mass-to-charge ratio of the target nucleus $K(Z)$, as a function of the nuclear charge; the dependence was obtained by Eq. (12). This curve can be extrapolated by the dependence

$$K(Z) \sim \frac{1}{\beta^2}\ln\left(\frac{\text{const}}{Z^2}\right). \tag{16}$$

As follows from Fig. 1, substituting the curve with a straight line $K(Z) = 18/\beta^2$ is not entirely acceptable for light and heavy targets.

According to the Bethe formula, targets with close values of Z should also have close values of mass RL. For example, it can be seen from Table 1 that the elements with $Z = 13$ (aluminum) and $Z = 14$ (silicon) have virtually the same calculated values of mass RL (1.53 and 1.56 MeV×(cm^2/g), respectively). However, it was experimentally confirmed in Ref. [14] that RL in silicon are higher than in aluminum by almost 1.5 times (1.5 and 2.1 MeV·(cm^2/g), respectively). Possible explanations for this difference may lie in the mechanism of internal ionization in semiconductors.

Table 1

Mean ionization potentials, mass RL, and coefficients for converting absorbed dose to fluence (and vice versa) for irradiation of different materials used in modern semiconductor electronics with 0.9 MeV electrons

Target material	I	$(1/\rho)\cdot(dE/dx)$	F/D
	eV	MeV·(cm^2/g)	1/Gy·cm^2
Graphene	69	1.72	$3.6\cdot10^9$
Aluminum	150	1.53	$4.1\cdot10^9$
Silicon	161	1.56	$4.0\cdot10^9$
Germanium	288	1.29	$4.8\cdot10^9$
Gold	711	1.04	$6.0\cdot10^9$

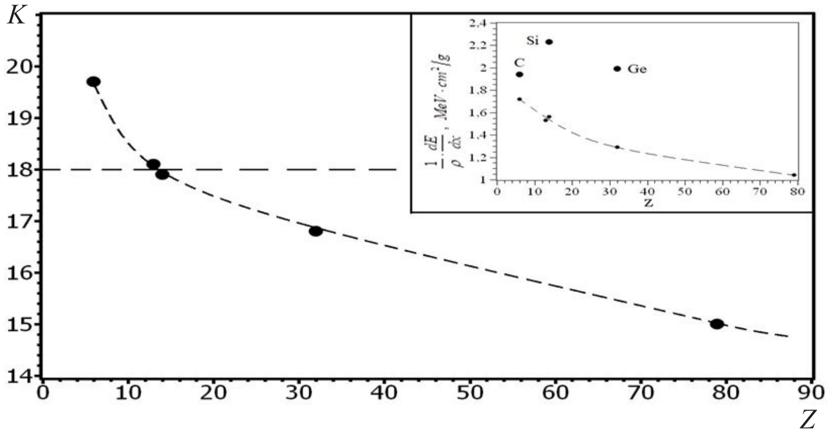

Fig. 1. Mass RL normalized to mass-to-charge ratio of target nucleus *K*(*Z*) as a function of nuclear charge; obtained by Eq. (12).
The inset shows mass RL as a function of the nuclear charge calculated by Eq. (11) within the Born approximation of scattering theory. The black dots indicate mass RL values obtained taking into account the internal ionization for graphene, silicon, and germanium

Contribution from internal ionization of semiconductors to radiative energy losses of relativistic electrons

The concept of internal ionization is introduced for condensed matter. Internal ionization in semiconductors and dielectrics corresponds to the transition of valence electrons to the conduction band (band-to-band transition). Klein [15] suggested an equation relating the energy for production of an electron-hole pair E_i and the band gap E_g (in eV):

$$E_i = 2.67E_g + 0.87, \tag{17}$$

establishing that the internal ionization energy is approximately three times more than the band gap.

E_i is higher than E_g because the energy of relativistic electrons is spent not only for ionization but also for generation of excited states in a solid, i.e., plasmons and phonons. Table 2 gives the energies E_i and E_g for the main materials used in modern semiconductor electronics (silicon, germanium) and graphene.

Since the average ionization potential, which is equal to ~9*Z* for most elements, is significantly (by orders of magnitude) higher than the energy for the production of electron-hole pairs in semiconductors, the main result of electron stopping is a sharp increase in the concentration of charge carriers. Mass RL are estimated by substituting into Eq. (10) the energies for production of electron-hole pairs for the materials

Table 2

Band gap, energy for production of electron-hole pairs, mass RL and pair production rate by single relativistic electron for three semiconductor materials

Target material	E_g	E_i	$(1/\rho)\cdot(dE/dx)$	$N_{e\text{–}p}/F$
	eV		MeV·(cm²/g)	cm⁻¹
Graphene	5.2	18.7	1.94	$1.6\cdot10^5$
Silicon	1.12	3.6	2.23	$1.4\cdot10^6$
Germanium	0.67	2.9	1.99	$3.7\cdot10^6$

listed in Table 2. The results obtained are given in column 3 of Table 2. Comparing the data in Table 1 and Table 2, we can conclude that taking into account internal ionization changes (that is, increases) the capacities for RL: for example, by almost 50 % for silicon and germanium (up to 2.23 MeV·(cm^2/g)).With this factor taken into account, the calculated values of mass RL (2.23 MeV·(cm^2/g)) are much closer to the experimental ones (2.21 MeV·(cm^2/g)) [14]. The black dots in the inset at Fig. 1 correspond to the values of mass RL normalized to mass-to-charge ratio of the target nucleus, accounting for internal ionization for graphene, silicon, and germanium. Let us estimate the concentration of electron-hole pairs produced by a single relativistic electron (N_{e-p}/F), dividing linear RL by pair production energy. This data is given in column 4. For example, this value for silicon is $1.4\cdot10^6$ cm^{-1}. Let us estimate the production rate of electron-hole pairs for the real electron accelerator running at Peter the Great St. Petersburg Polytechnic University. Irradiation with electrons is performed using an RTE-1V pulse accelerator. Pulse frequency is 450 Hz, pulse duration 370 μs, duty cycle 1/6. A beam with a current of 1 mA and a cross-sectional diameter of 0.9 cm scans over an area of 2 × 40 cm. The mean current density of the beam during irradiation with electrons is taken to be 12.5 μA·cm^{-2}; however, the current density in the pulse is much higher, reaching 6 mA·cm^{-2}. The electron flux density in the pulse at such currents is $3.6\cdot10^{16}$ cm^{-2}s^{-1}, and the total production rate for electron-hole pairs upon electron irradiation reaches a huge value ($1.4\cdot10^6\cdot3.6\cdot10^{16}$) = $= 5\cdot10^{22}$ cm^{-3}s^{-1}. An additional charge is generated upon irradiation of MOS structures and field-effect transistors at the insulator-semiconductor interface and in the bulk of the insulator due to production of electron-hole pairs, resulting in a change in the main characteristic, which is the threshold voltage of the device [9].

Summary

The results obtained in the course of our investigation led us to the following conclusions:

1. Accounting for internal ionization of semiconductors due to production of electron-hole pairs changes (increases) the stopping powers of relativistic electrons, for example, by almost 50% for silicon and germanium.
2. This in turn offers a consistent explanation for the values of mass RL observed experimentally.
3. The analysis carried out in the study should allow making more effective and more detailed predictions for the performance of semiconductor devices in real conditions, particularly, in space.

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