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Energy-loss dependence of inelastic interactions between high-energy electrons and semiconductors: a model to determine the spatial distribution of electron–hole pairs generation

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Abstract

A scattering model to evaluate the extent of generated electron–hole pairs (e–h) in semiconductors during electron beam excitation in the 5–40 keV beam energy range is presented. From a modified Kanaya and Okayama model, the range R and energy-loss equation dE/dS dependence on the inelastic and elastic scattering cross-section proportion are analytically deduced. The presented model allows to modulate the proportion of inelastic–elastic scattering cross-section versus the energy of the incident electrons as occurs for each different interaction. Into this formalism is introduced the rate of Kα ionization events at different incident electron energy. This model is then used in Monte Carlo calculations to deduce the e–h generation function $g(x, y, z)$ at different electron beam energy (E_b) levels. As a result, both depth and lateral dependences of e–h generation are found to fit successfully the experimental distributions of Bonard et al. (*J. Appl. Phys., 79* (1996) 8693.

Keywords: Semiconductors; Electron–hole pairs; Scattering model

1. Introduction

In recent decades, the study of the interaction between high-energy electrons and semiconductors has attracted great interest either for its fundamental physics [1] or for its applications in detectors and scanning electron microscopy (SEM) modes characterization [2–4]. Indeed, the spatial resolution of the electron-beam-induced current (EBIC) and cathodoluminescence (CL) modes is first of all dependent on the extent of the generated electron–hole pairs (e–h) during the SEM electron beam excitation and secondly on the diffusion of such a generated e–h. Hence, the EBIC and CL quantitative analysis requires an understanding of the physics of this interaction.

The most commonly used approach consists in applying the Rutherford cross-section to determine scattered electron deflections and the Bethe energy-loss equation for its energy transfer [5–7]. Recently, Bonard et al. [8] demonstrated that this Rutherford–Bethe physical frame predicts only an acceptable e–h generation distribution in a limited range of electron beam energy. A discrepancy between the experimental and theoretical/empirical predictions [2] is evidenced for beam energies $E_b < 10$ keV and $E_b > 20$ keV. The reasons for this discrepancy are discussed here. The key reason for this discrepancy is the dependence on the incident electron energy of each elastic and inelastic scattering process that can never be evaluated. However, as a first approximation (using a Kanaya and Okayama-based formalism [9]), we introduce the total inelastic scattering cross-section contributions versus elastic scattering ones, represented by the numerical parameter s, that is here determined versus the beam energy. The analytical R and dE/dS expressions are then introduced in Monte Carlo computational algorithms to estimate both depth and lateral generated e–h distributions at different electron beam energies, that are found to fit successfully the Bonard et al. experimental distributions of generated e–h for $Al_{0.4}Ga_{0.6}As$. Therefore, this calculated e–h generation function $g(x, y, z)$ may be used for EBIC and CL

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quantitative analysis [10]. The proposed model can be straightforwardly applied to other III-V and II-VI semiconductors.

2. The Kanaya and Okayama scattering model

The quasi-elastic scattering theory of Kanaya and Okayama [9], based on the Lindhard theory, describes the interaction between high-energy beam electrons and atoms through the screened potential $V(r) = Ze^2a^{s-1}/sr^s$, with $a = \kappa_{TF}a_H Z^{-1/3}$, where Z is the atomic number of interacting atoms, e the electronic charge and a the effective screened atom radius. κ_{TF} is the Thomas–Fermi constant and a_H the hydrogen atom Bohr radius. In these expressions, s is a numerical parameter related to the screening by bounded electrons and is therefore directly dependent on the inelastic scattering cross-section σ_e contribution with respect to the elastic one σ_n ($s = 1$ corresponds to Rutherford scattering cross-sections) in scattering events. From experimental estimations Kanaya and Okayama evaluated $s = 6/5$.

The Kanaya and Okayama nuclear (elastic) scattering cross-section is thereby expressed by

$$\sigma_n = \lambda_s \frac{3.33\pi 2^{11/6} a^{1/3} e^{10/3} Z^{5/3}}{4E^{5/3}}, \qquad (1)$$

where λ_s is a constant determined experimentally ($\lambda_s = 0.182$). The factor 3.33 results in the integration of the differential nuclear scattering cross-section dependence of the angular scattering, taking into account multiple scattering events. The Kanaya and Okayama energy-loss equation from inelastic scattering events results in

$$\frac{dE}{dS} = \lambda_s \frac{3\pi 2^{5/3} a^{1/3} e^{10/3} Z}{E^{2/3}} \frac{N_A \rho}{A}, \qquad (2)$$

where N_A is the Avogadro number, ρ the semiconductor density and A its atomic weight. The range R or maximum penetration depth may be deduced from energy-loss Eq. (2):

$$R = \int_0^{E_b} \frac{dE}{dE/dS} = \frac{E_b^{5/3}}{\lambda_s 5\pi 2^{5/3} a^{1/3} e^{10/3} Z} \frac{A}{N_A \rho}, \qquad (3)$$

with E_b as the electron beam energy.

3. Results and discussion

3.1. The s-scattering model

During SEM electron beam excitation, the energy-loss by inelastic scattering events involves multiple processes in semiconductors (plasmons, phonons, secondary electrons, inner-shell ionization, 'bremsstrahlung', electron–hole pairs generation). Each process involved depends on the incident electron energy. This means that the proportion of inelastic–elastic events varies with the electron energy. Therefore, the numerical parameter s is not a constant value but rather a function of E_b. We suggest a modified Kanaya and Okayama scattering model, introducing the inelastic scattering cross-section contribution to scattering events as dependent on beam energy, i.e., s:$s(E_b)$.

From Kanaya and Okayama, the differential electronic (inelastic) scattering cross-section dependence on s results in:

$$d\sigma_e = \lambda_s \frac{2^{2/s-1}\pi a^{2-2/s} e^{4/s}}{E^{2/s}} \frac{T_m^{1/s}}{T^{1+1/s}} dT, \qquad (4)$$

where T and T_m are the transferred energy and its maximum value. The energy-loss equation dE/dS derived from the differential inelastic scattering cross-section is deduced as follows:

$$\frac{dE}{dS} = \frac{N_A\rho}{A} Z \int_0^{T_m} T \frac{d\sigma_e}{dT}$$
$$= \lambda_s \frac{\pi a^2}{2} \frac{s}{s-1} \frac{N_A \rho}{A} Z^{(2+s)/3s} \left(\frac{2e^2}{a}\right)^{2/s} E^{1-2/s} \qquad (5a)$$

for $s > 1$, and

$$\frac{dE}{dS} = \lambda_s \pi \frac{N_A\rho}{A} 2Ze^4 \frac{1}{E} \ln(E) \qquad (5b)$$

for $s = 1$.

The range R may be analytically deduced from Eq. (5a):

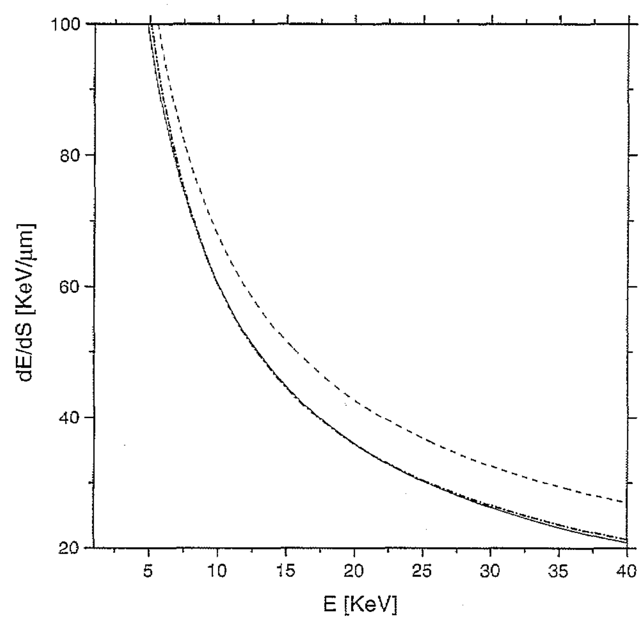

Fig. 1. Comparison of the energy-loss equations dE/dS from Bethe (——) and Kanaya and Okayama (– – –), with $s = 6/5$ and $\lambda_s = 0.182$. The Bethe expression is confronted with the energy-loss Eq. (5). The closest fit corresponds to $s \approx 8/7$ and $\lambda_s = 0.168$ (– · –).

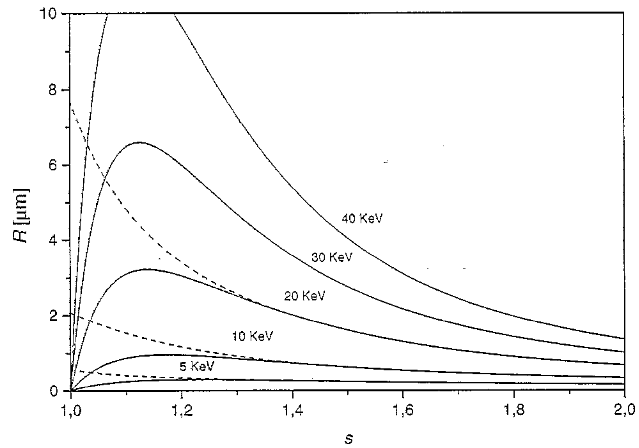

Fig. 2. Range R vs. the numerical parameter s at different electron beam energies in the 5–40 keV range (——). The exponential-like behaviour of $R(s)$ using $R(s=1)$ calculated value is represented by (- - -).

$$R=\int_0^{E_b}\frac{dE}{dE/dS}=\frac{(s-1)A}{\rho\lambda_s\pi a^2\left[\frac{2e^2}{a}\right]^{2/s}N_A Z^{(2+s)/3s}}E_b^{2/s} \quad (6)$$

for $s>1$, whereas for $s=1$, R must be calculated by numerical methods.

The parameter λ_s is estimated by comparison between the energy-loss Eq. (5) and the Bethe one. The Bethe energy-loss equation must be a particular solution of Eq. (5). Therefore, s and λ_s may be determined. Indeed, Fig. 1 shows the energy-loss versus the electron energy. Both expressions lead to identical energy-loss dependences if $s\approx 8/7$ and $\lambda_s=0.168$. Hence, both parameters are analytically deduced here.

Fig. 2 displays the predicted range R versus the numerical parameter s for varying electron beam energies in the range 5–40 keV (——). As a consequence of the $(s-1)$ factor in Eq. (6), R tends to zero closest to $s=1$. Nevertheless, for $s=1$ this equation may not be applied and the depth of maximum penetration must be evaluated by numerical methods through Eq. (5b). Therefore, a discontinuity occurs at $s=1$. To overcome the $s\rightarrow 1$ peculiarity, we replace Eq. (6) by an exponential-like behaviour of R versus s represented by (– – –).

An evaluation of the s dependence on electron beam energy $s(E_b)$ is possible, confronting such results with the most reliable experimental data of Bonard et al. for $Al_{0.4}Ga_{0.6}As$. Fig. 3 shows the function $s(E_b)$ in the 1–40 keV electron beam energy range. For $E_b>10$ keV, $s=1.308$, a constant value, but for $E_b<10$ keV, s decreases strongly towards unity. This s versus E_b behaviour fits successfully a sigmoidal (Fermi–Dirac-like) function:

$$s(E_b)=\frac{s_1-s_2}{1+\exp\left(\frac{E_b-E_{cut-off}}{\varepsilon}\right)}+s_2, \quad (7)$$

where $s_1=1$, $s_2=s(E_b)_{10\ keV}\approx 1.308$, $\varepsilon\approx 1.2$ keV and $E_{cut-off}\approx 7.7$ keV. $E_{cut-off}$ may be related to the ionization energies of the K-shell (Lyman series) and its corresponding ionization rate. Indeed, $E_{cut-off}$ coincides numerically with Kα (7658 eV) for $Al_{0.4}Ga_{0.6}As$, assumed as like-element of $Z=28.4$.

Hence, at electron beam energies over the Lyman series, the inelastic scattering cross-section contribution to scattering events is approximately constant. Nevertheless, for $E_b>10$ keV, s decreases strongly towards $s=1$, giving us to understand that inelastic scattering phenomena decrease strongly. The ionization of inner-shells (relaxed to X-ray and Auger emissions) is the maximum energy transference process. As a consequence of the fact that Kα ionizations do not occur down cut-off energies, energy transference is leading to other processes, such as e–h generation.

3.2. The Monte Carlo method

Our Monte Carlo procedures are based on the multiple-scattering Monte Carlo model assumptions [6]. The range R may be calculated from the above proposed s-scattering model. R is then divided into computational steps to compute the scattering coordinates (x, y, z) and energy-loss distributions. The electron beam energy at the i-step is estimated by

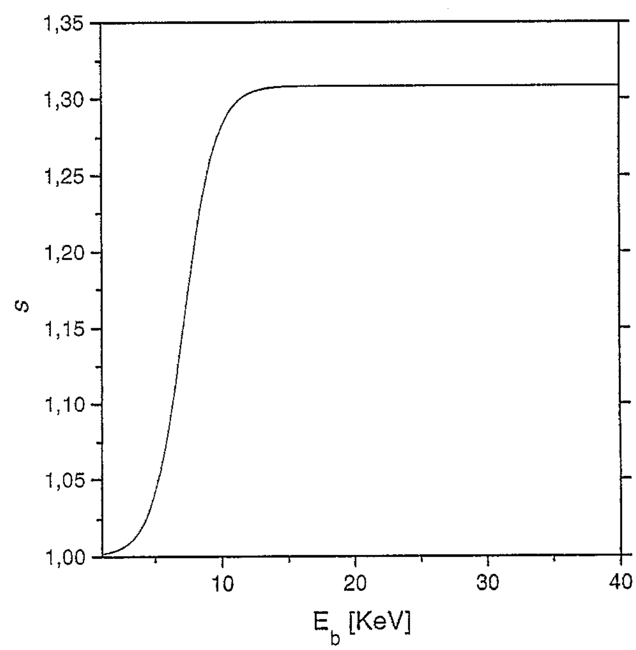

Fig. 3. The s-dependence of electron beam energy E_b in the 1–40 keV range; s diminishes strongly for $E_b<10$ keV because of K-shell ionization rate cut-off. The inelastic vs. elastic cross-section proportion changes down 10 keV due to the impossibility of reaching K-ionization below this energy.

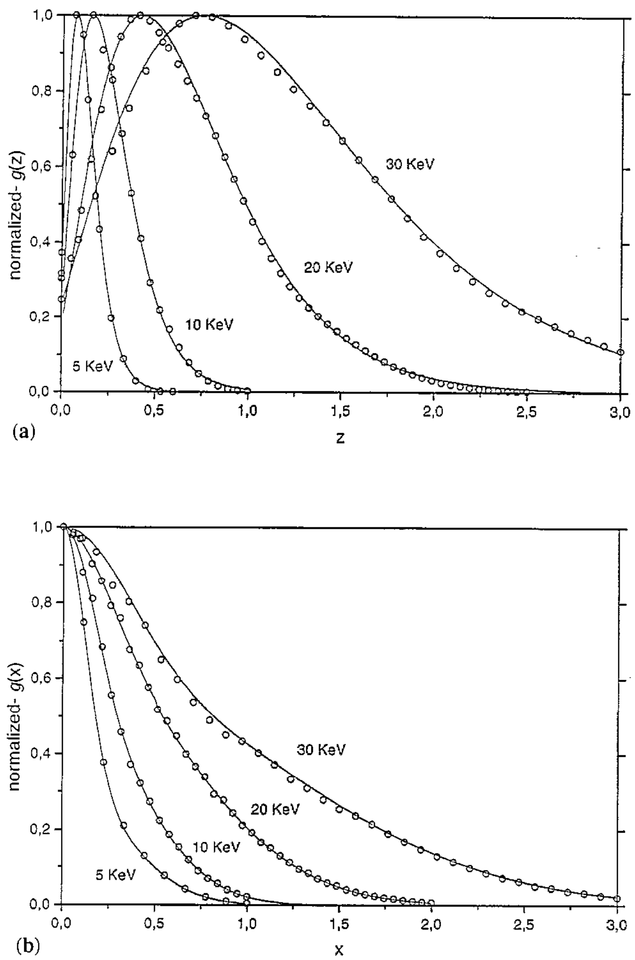

Fig. 4. Depth (a) and lateral (b) distributions of generated electron–hole pairs at different beam energies of 5, 10, 20 and 30 keV: the predicted Monte Carlo values (O) are shown to fit very well the analytical functions of Bonard et al. (——).

$$E(i) = E(i-1) - \int_{\text{step}} (\mathrm{d}E/\mathrm{d}S)\,\mathrm{d}S. \tag{8}$$

The scattering angle ϕ is evaluated at each computational step through $\tan(\phi/2) = B \times \mathrm{Rnd}/E(i)$ suggested by Akamatsu et al. [11], where B is a numerical parameter adjusted to obtain the backscattering coefficient and Rnd is a uniformly distributed random number ($\mathrm{Rnd} \subset [0, 1]$). The number n of e–h generated along the i-step is computed as $g(x, y, z) = [E(i-1) - E(i)]/E_{\text{e–h}}$, where $E_{\text{e–h}}$ is the energy of an electron–hole pair generation [12]. Therefore, the depth and lateral distributions of generated e–h are calculated, respectively, by

$$g(z) = \frac{1}{\gamma}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} g(x, y, z)\,\mathrm{d}x\,\mathrm{d}y \tag{9a}$$

and

$$g(x) = \frac{1}{\gamma}\int_{0}^{+\infty}\int_{-\infty}^{+\infty} g(x, y, z)\,\mathrm{d}y\,\mathrm{d}z, \tag{9b}$$

where γ is a normalization factor. Fig. 4(a) displays both calculated and measured [8] depth distributions for electron beam energies of 5, 10, 20 and 30 keV. Their corresponding lateral dependences are shown in Fig. 4(b). A good agreement between experimental and theoretical predictions based on the presented scattering model are found in the SEM working electron beam energy range.

4. Conclusion

A model to estimate the spatial distribution of the generated electron–hole pairs during SEM electron beam excitation of semiconductors is presented. The scattering formulation involves, for the first time, the proportion of inelastic–elastic cross-sections that is applied to the incident electron energy dependence of the Kα-shell ionization. The result is a very good agreement of the e–h generation distributions with recently published experimental measurements of the pear-shaped volume of generation in $Al_{0.4}Ga_{0.6}As$.

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