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A New Model Formulation for Electron Interactions in Ge

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Abstract: A Monte Carlo model that simulates the primary electron production inside the photoconductors mentioned, for a number of monoenergetic and polyenergetic x-ray spectra that cover the mammographic energies has been developed. The model simulates the primary photon interactions (photoelectric absorption, coherent and incoherent scattering) as well as the atomic deexcitations (fluorescent photon production, Auger and Coster-Kronig electron emission). In addition, a mathematical formulation has been developed for the drifting of primary electrons of a-Ge in vacuum under the influence of a capacitor's electric field and the electron characteristics on the collecting electrode are being studied. The formulation is based on the Newton's equations of motion and the theorem for kinetic energy change. Furthermore, a code has been developed that calculates the distribution of the electric potential inside a-Ge using an existing analytical solution, the boundary values of the case and certain numerical calculation methods. Finally, the structure and the mathematical formulation of a model that would simulate the electron interactions inside a-Ge have been developed. An existing model has been reexamined and enriched with certain theoretical considerations and simulation formalisms.

Key words: Monte Carlo, Auger, Coster-Kronig, electron, solution, electrode

INTRODUCTION

The x-ray induced primary electrons inside the photoconductor's bulk comprise the primary signal that propagates in the material and forms the final signal (image) at the detector's electrodes. As the signal propagates, electrons interact with the material and are subject to recombination and trapping. Lachaine, Fallone and Fourkal have dealt with the signal propagation inside a-Se.

In particular, Lachaine and Fallone (Bloomquist *et al*., 2006; Choquette *et al*., 2001) made calculations on the electron inelastic scattering cross-sections as well as Monte Carlo simulations of x-ray induced recombination. Davisson and Evans (1952), Green *et al*. (1988), Haugen *et al*. (1999) and Jahnke and Matz (1999) made a complete simulation of the signal formation in a-Ge. The formulations were based on theoretical calculations mainly developed by Ashley (Green *et al*., 1988; Kasap *et al*., 2004; Morin, 1998; Pang *et al*., 1998; Rowlands *et al*., 1992; Jr Saunders *et al*., 2004; Su *et al*., 2005; Zhao *et al*., 1998).

During this PhD thesis the model of Fourkal has been reexamined and enriched with existing theoretical considerations and simulation formalisms. This study presents the structure and the mathematical formulation of a model that would simulate the electron interactions inside a-Ge.

Electron free path length: The free path length between two successive electron interactions is assumed to obey Poisson statistics.

Thus the probability density function for the free path length s is:

$$P(s) = \lambda_{tot}^{-1} e^{-\frac{s}{\lambda_{tot}}} \quad (1)$$

where, λ_{tot} is the total mean free path. The number of molecules (atoms) per unit volume is:

$$N = N_A \frac{\rho}{A_M} \quad (2)$$

Where:

N_A = The Avogadro's number
A_M = The molecular weight
ρ = The density

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The electrons are assumed to undergo only elastic and inelastic scatterin. Thus, the total interaction cross section is defined as:

$$\sigma_{tot}(E) = \sigma_{el}(E) + \sigma_{inel}(E) \quad (3)$$

where, σ_{el} and σ_{inel} are the elastic and inelastic scattering cross sections, respectively. Thus, the mean free path is defined as:

$$\lambda_{tot} = \frac{1}{N\sigma_{tot}} \quad (4)$$

Decision on the type of electron interaction: From equation it is derived that:

$$\frac{\sigma_{el}}{\sigma_{tot}} + \frac{\sigma_{inel}}{\sigma_{tot}} = 1$$

If the probabilities for elastic (P_{el}) and inelastic (P_{inel}) scattering are defined as:

$$P_{el} = \frac{\sigma_{el}}{\sigma_{tot}} \quad (5)$$

$$P_{inel} = \frac{\sigma_{inel}}{\sigma_{tot}} \quad (6)$$

Then a random decision is made based on P_{el} and P_{inel} to determine the type of electron interaction process.

ELASTIC SCATTERING

Differential cross section: The theory of elastic scattering has been discussed elsewhere (Bloomquist *et al*., 2006).

Since we work in non-relativistic electron energies where the exchange and polarization effects are negligible, the Mott differential cross section can be written as Salvat:

$$\frac{d\sigma_{el}}{d\Omega} = |f(\theta)|^2 \quad (7)$$

Where:

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta l} - 1)P_l(\cos\theta) \quad (8)$$

As it is stated by Salvat the scattering amplitude $|F(\theta)|^2$ can be calculated by using the first Born approximation and some additional concepts to compensate for the fact that the Born cross section is not valid for small electron energies. Within the range of validity of the Born approximation that is for relatively large energies of the incident electron (500 eV-50 keV), the Born (B) scattering amplitude is given by (for a measuring system with m = e = 1):

$$f^{(B)}(\theta) = -2\int_0^{\infty}\frac{\sin(qr)}{qr}V(r)r^2dr \quad (9)$$

where, q = 2k sin(θ/2) is the momentum transfer. Equation can be written as:

$$f^{(B)}(\theta) = \frac{1}{2ik}\sum_{l=o}^{\infty}(2l+1)2i\delta_l^{(B)}P_l(\cos\theta) \quad (10)$$

With the phase shifts:

$$\delta_l^{(B)} = -2k\int_0^{\infty}V(r)(j_l(kr))^2r^2dr \quad (11)$$

where, j_l (kr) are spherical Bessel functions. Salvat assume that:

$$f(\theta) = f^{(B)}(\theta) + \underbrace{\sum_l F(\theta, \delta_l^{(B)}, \delta_l)}_{\text{correction}} \quad (12)$$

With

$$F(\theta, \delta_l^{(B)}, \delta_l) = \frac{1}{2k}(2l+1)(\sin 2\delta_l - 2\delta_l^{(B)} + i(1-\cos 2\delta_l))P_l(\cos\theta) \quad (13)$$

If an analytical screened Coulomb potential is assumed of the form:

$$V_{an}(r) = -\frac{Z}{r}\left[Ae^{-a_1r} + (1-A)e^{-a_2r}\right] \quad (14)$$

where, A, α_1 and α_2 are constants that characterize the material then Eq. 11 becomes:

$$f_{an}^{(B)}(\theta) = 2Z\left(\frac{A}{a_1^2+q^2} + \frac{1-A}{a_2^2+q^2}\right) \quad (15)$$

and the phase shifts become:

$$\delta_{l,an}^{(B)} = \frac{Z}{k}\left[AQ_l\left(\frac{a_1^2}{2k^2}+1\right) + (1-A)Q_l\left(\frac{a_2^2}{2k^2}+1\right)\right] \quad (16)$$

where, Q_l are the Legendre functions of the second kind. Therefore, from Eq. 15 using Eq. 10-12 and additional calculating ideas Salvat calculate the elastic scattering cross section.

For the sake of simplicity, it can be assumed that even for low electron energies the Born approximation is valid and therefore (15) becomes $f(\theta)\approx f^{(B)}(\theta)$. Using this assumption equation can be written as:

$$\frac{d\sigma}{d\Omega}=\left|f_{an}^{(B)}(\theta)\right|^2=\left|2Z\left(\frac{A}{a_1^2+q^2}+\frac{1-A}{a_2^2+q^2}\right)\right|^2\Rightarrow$$

$$\frac{d\sigma}{d\theta}=2\pi\sin\theta\left|2Z\left(\frac{A}{a_1^2+q^2}+\frac{1-A}{a_2^2+q^2}\right)\right|^2 \quad (17)$$

Taking into account that $q = 2k \sin(\theta/2)$ and that for the non-relativistic case $k=\sqrt{2mE}/\hbar$ we get:

$$\frac{d\sigma}{d\theta}=2\pi\sin\theta\left|2Z\left(\frac{A}{a_1^2+\left(2k\sin\left(\frac{\theta}{2}\right)\right)^2}+\frac{1-A}{a_2^2+\left(2k\sin\left(\frac{\theta}{2}\right)\right)^2}\right)\right|^2\Rightarrow$$

$$\frac{d\sigma}{d\theta}=2\pi\sin\theta\left|2Z\left(\frac{A}{a_1^2+4\left(\frac{\sqrt{2mE}}{\hbar}\sin\left(\frac{\theta}{2}\right)\right)^2}+\frac{1-A}{a_2^2+4\left(\frac{\sqrt{2mE}}{\hbar}\sin\left(\frac{\theta}{2}\right)\right)^2}\right)\right|^2\Rightarrow$$

$$\frac{d\sigma}{d\theta}(S.I.)=\frac{8\pi Z^2}{a_0^2}\sin\theta\left(\frac{A}{a_1^2+\frac{8m}{\hbar^2}E\sin^2\left(\frac{\theta}{2}\right)}+\frac{1-A}{a_2^2+\frac{8m}{\hbar^2}E\sin^2\left(\frac{\theta}{2}\right)}\right)^2 \quad (18)$$

With $a_0 = \hbar^2/me^2$ and $A = 0.4836$, $\alpha_1 = 8.7824$, $\alpha_2 = 1.6967$ for a-Se Salvat. The elastic scattering angle θ of the electron can be sampled from Eq. 17 using the rejection method:

Elastic scattering cross section (σ_{el}): The elastic scattering cross section is given by:

$$\sigma_{el}=\int\frac{d\sigma_{el}}{d\Omega}d\Omega=\int\frac{d\sigma_{el}}{d\theta}d\theta=\int\frac{d\sigma_{el}}{dq^2}dq^2 \quad (19)$$

Using equation, $q = 2k \sin(\theta)/2$ and $d\Omega = 2\pi\sin\theta d\theta$ we calculate that:

$$\frac{d\sigma}{dq^2}=\frac{4Z^2}{a_0^2k^2}\left(\frac{A}{a_1^2+q^2}+\frac{1-A}{a_2^2+q^2}\right)^2 \quad (20)$$

Since $q^2 = (2k \sin(\theta/2))^2$ when $\theta = 0$, $q^2 = 0$ and when $\theta = \pi$, $q^2 = 4k^2$. Thus Eq. 20 is written as:

$$\sigma_{el}=\int_0^{4k^2}\frac{4Z^2}{a_0^2k^2}\left(\frac{A}{a_1^2+q^2}+\frac{1-A}{a_2^2+q^2}\right)^2dq^2 \quad (21)$$

Calculating the integral we find that:

$$\sigma_{el}=\frac{4Z^2}{a_0^2k^2}\times\left(\begin{array}{l}\frac{-A^2}{a_1^2+4k^2}-\frac{(1-A)^2}{a_2^2+4k^2}-\frac{2(1-A)A}{a_1^2-a_2^2}\ln\left[\frac{a_1^2+4k^2}{a_2^2+4k^2}\right]\\+\frac{A^2}{a_1^2}+\frac{(1-A)^2}{a_2^2}+\frac{2(1-A)A}{a_1^2-a_2^2}\ln\frac{a_1^2}{a_2^2}\end{array}\right) \quad (22)$$

with

$$k=\frac{\sqrt{2mE}}{\hbar}$$

INELASTIC SCATTERING

Inelastic scattering with inner shells (K and L shells): Fourkal state that the inelastic scattering events with inner shells are not affected by the physical state of the medium. Therefore they use tabulated cross sections for independent Se atoms from the Evaluated Electron Data Library (EEDL) of the Lawrence Livermore National Laboratory Cullen and Perkins. The EEDL:

- Gives the subshells ionization cross sections
- Gives the energy of the ejected secondary electrons
- Assumes that the direction of the incident electron is not changed during the interaction process. Thus angular distributions are not given
- Angular distributions of the secondary electrons are not given

Salvat state that during an inelastic scattering event with inner shell the correlation between energy loss/scattering of the projectile and ionization events is of minor importance and may be neglected. Consequently, the inner-shell ionization is considered as an independent interaction process that has no effect on the state of the projectile.

Accordingly, in the simulation of inelastic collisions with inner shells the projectile is assumed not to be deflected from its original direction but only cause the ejection of knock-on electrons (delta rays). From what it is mentioned above, it is obvious that the only quantity

that must be calculated is the energy loss W of the incident electron. Salvat have calculated the differential cross section for inelastic collisions with inner shells using a semiphenomenological approach. In this approach the relationship between the Optical Oscillator Strength (OOS) of ith inner shell with the photoelectric cross section for absorption of a photon with energy W from this shell, $\sigma_{ph,i}(Z,W)$ is:

$$\frac{df_i(W)}{dW} = \frac{mc}{2\pi^2 e^2 \hbar}\sigma_{ph,i}(Z,W) \quad (23)$$

This relationship holds when the dipole approximation is applicable i.e., when the wavelength of the photon is much larger than the size of the active shell. Following the formalism of Salvat, the generalized oscillator for ith inner shell is:

$$\frac{df_i(Q,W)}{dW} = \int_{B_i}^{\infty} \frac{df_i(W')}{dW'} F(W';Q,W)\, dW' + Z_r \delta(W-Q)\Theta(W-B_i) \quad (24)$$

with

$$F(W';Q,W) = \delta(W-W')\Theta(W'-Q) + \delta(W-Q)\Theta(Q-W') \quad (25)$$

$$Z_r = Z_i - \int_{B_i}^{\infty} \frac{df_i(W')}{dW'} dW' \quad (26)$$

and Θ being the step function, Z_i is the number of electrons of ith shell and B_i is the binding energy of the inner shell. Using Eq. 22 Salvat calculated the differential cross section for inelastic scattering with inner shells which for the case of non-relativistic energies is:

$$\frac{d\sigma_{inel}^{inner,i}(E)}{dW} = \frac{2\pi e^4}{mu^2}\left\{\frac{df_i(W)}{dW}\frac{1}{W}\ln\left(\frac{W}{Q_-}\right) + \left(Z_i - \int_W^{\infty}\frac{df_i(W')}{dW'}dW'\right)\frac{1}{W^2}F^{(-)}(E,W)\right\}\Theta(W-B_i)\Theta(W_{max}-B_i) \quad (27)$$

Where:

$$Q_- = (\sqrt{E} - \sqrt{E-W})^2 \quad (28)$$

$$F^{(-)}(E,W) = 1 + \left(\frac{W}{E-W}\right)^2 - \frac{W}{E-W} \quad (29)$$

Consequently the steps that must be followed to calculate the differential cross section are:

- Calculation of $df_i(W)/dW$ from (28)
- Setting the number of electrons in the ith subshell, Z_i
- Calculation of the integral by $\int_W^{\infty} df_i(W')/dW'\, dW'$ making a fit to the data of photoelectric cross section and integrating analytically
- Rejection method to sample the energy loss W of the incident electron

The Born approximation overestimates the differential cross sections for incident electrons with kinetic energies near the binding energy B_i. This is mainly due to the distortion of the projectile wave function by the electrostatic field of the target atom.

To account for this effect we assume that the incident electron gains a kinetic energy $2B_i$ and that $W_{max} = (E+B_i)/2$. The inelastic scattering cross section with inner shells is given by:

$$\sigma_{inel}^{inner,i} = \int_{B_i}^{(E+B_i)/2} \frac{d\sigma(E+2B_i)}{dW} dW \quad (30)$$

The Coulomb correction reduces the differential cross section near the threshold B_i and yields values in better agreement with the experimental data.

Inelastic scattering with outer shells: The model of Fourkal for simulating the inelastic collisions of electrons with outer shells is based on a theory developed by Ashley. Some comments for this model are given below:

- It is a semi-empirical one and describes the inelastic interactions of low energy electrons with condensed matter in terms of the optical properties of the considered medium
- It is a statistical model: the stopping medium is viewed as an inhomogeneous electron gas and the Differential Inverse Mean Free Path (DIMFP) is obtained as an average of the DIMFPs in free electron gases of different densities. Weights are used to average the free electron gas's DIMFPs with the incorporation of experimental optical dielectric data
- It is not a relativistic one
- Ashley uses experimental OOSs and accounts for exchange effects
- The model leads to realistic results for low energy electrons i.e., when the majority of excitations correspond to the outer shells. The model is notsuitable for describing inner-shell ionizations

The complex dielectric function $\epsilon(q,w)$ gives the response of a medium to a given energy transfer W and momentum transfer q.

The medium is assumed to be homogeneous and isotropic so that ϵ is a scalar quantity and not a tensor. The probability of an energy loss W per unit distance traveled by a non-relativistic electron of energy E is (in atomic units i.e., $\hbar = m = e = 1$):

$$\tau(E,W) = \frac{1}{\pi E}\int_{q-}^{q+}\frac{dq}{q}\,\mathrm{Im}\left\{\frac{-1}{\epsilon(q,W)}\right\} \tag{31}$$

With

$$q_{\pm} = \sqrt{2}\left[\sqrt{E} \pm \sqrt{E-W}\right]$$

This expression for $q_{\pm}$ assumes that the energy-momentum transfer relation for the electron moving in the medium is the same as that for a free electron in vacuum.

The extension of the energy loss function to q>0 from the optical limit is made through:

$$\mathrm{Im}\left[\frac{-1}{\epsilon(q,W)}\right] = \int_0^{\infty} dW'\,\frac{W'}{W}\,\mathrm{Im}\left[\frac{-1}{\epsilon(0,W')}\right]\delta\left(W-\left(W'+\frac{q^2}{2}\right)\right) \tag{32}$$

The energy loss sum rule is:

$$\int_0^{\infty} dW W\,\mathrm{Im}\left[\frac{-1}{\epsilon(q,W)}\right] = 2\pi^2 n_0 Z \tag{33}$$

With n_0 being the density of atoms or molecules in the medium with Z electrons per atom or molecule. The quantity W' is called binding energy but it has nothing to do with the binding energy of electrons in atomic shells. Its meaning will be discussed later on. Eq. 32 using 33 becomes:

$$\tau(E,w) = \frac{1}{2\pi E}\int_0^{\infty} dW' W'\,\mathrm{Im}\left[\frac{-1}{\epsilon(0,W')}\right]F(E,W',W) \tag{34}$$

with

$$F(E,W',W) = \frac{\Theta\left(W-\frac{q_-^2}{2}-W'\right)\Theta\left(W'-W+\frac{q_+^2}{2}\right)}{W(W-W')} \tag{35}$$

Equation 34 can be rewritten including exchange effects and indistinguishability as:

$$\tau_{exc}(E,w) = \frac{1}{2\pi E}\int_0^{\infty} dW' W'\,\mathrm{Im}\left[\frac{-1}{\epsilon(0,W')}\right]\times \left\{\overbrace{F(E,W',W)+F(E,W',E+W'-W)}^{\text{indisthguishability}} - \overbrace{\left[F(E,W',W)F(E,W',E+W'-W)\right]^{1/2}}^{\text{exchange}}\right\} \tag{36}$$

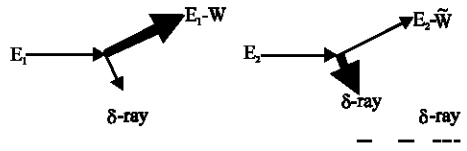

Fig. 1: Schematical illustration of the indistinguishability between a scattered projectile with energy E1-W and a secondary electron (δ-ray) with the same energy

The exchange effects concern spin interactions. The indistinguishability can be understood as follows: an energy transfer W by the primary electron reducing its energy to E-W gives an electron which cannot be distinguished from the secondary electron of energy E-W produced by a different energy transfer from the primary electron to the struck electron. Figure 1 shows this situation schematically. The Ashley's approximation 34 can be rewritten as follows (S.I):

$$\mathrm{Im}\left\{\frac{-1}{\epsilon(q,W)}\right\} = \int_0^{\infty} dW'\,\frac{W'}{W}\,\mathrm{Im}\left\{\frac{-1}{\epsilon(0,W')}\right\}\delta\left(W-\left(W'+\frac{\hbar q^2}{2m}\right)\right) = \int_0^{\infty}\frac{dBf(B)}{E'}\,\delta\left(E'-\left(B+\frac{\hbar^2 q^2}{2m}\right)\right) \tag{37}$$

where, f(B) is the OOS, E' = ħW is the energy loss and B = ħW' is the previously mentioned binding energy. The physical meaning of B that is of W' can be understood from the following equation:

$$E' = B + \frac{\hbar^2 q^2}{2m} \tag{38}$$

Where the term $\hbar^2q^2/2m$ is the kinetic energy of a free and initially at rest electron that acquires momentum q. The region of integration on (E', B) plane is formed from the following constrains:

$$\begin{cases} E' \le \frac{1}{2}(E+B)\ \text{(Energy conservation)} \\ E' \ge \frac{1}{2}\left(E+B-\sqrt{E(E-2B)}\right)\ \text{(Momentum conservation)} \end{cases}$$
$$B \ge 0 \tag{39}$$

Therefore the differential cross section for energy loss E in inelastic scattering with an outer shell is derived from Eq. 38:

$$\frac{d\sigma}{dE'} = \sigma'(E,E') = \chi\int_{\max(0,2E'-E)}^{2E'-E+2\sqrt{E(E-E')}} dBf(B)G(E,E',B) \tag{40}$$

with

$$\chi = \frac{\pi e^4}{(4\pi\varepsilon_o)^2} E \tag{41}$$

$$G(E,E',B) = \frac{1}{E'(E'-B)} + \frac{1}{(E-E')(E+B-E')} - \sqrt{\frac{1}{E'(E'-B)(E-E')(E+B-E')}} \tag{42}$$

The inelastic scattering cross section for energy loss E' is:

$$\sigma_{inel}^{outer}(E) = \int_0^{\frac{3E}{4}} \frac{d\sigma}{dE'} dE' \Rightarrow \sigma_{inel}^{outer}(E) = \chi \int_0^{\frac{E}{2}} dB f(B) P(E,B) \tag{43}$$

Where:

$$P(E,B) = \frac{1}{B} \ln\left(\frac{(E+B-S)(E-B+S)}{(E-B-S)(E+B+S)}\right) - \frac{2}{E+B} F\left(\sin^{-1}\left(\frac{S}{E-B}\right), \frac{E-B}{E+B}\right) \tag{44}$$

$$S = \sqrt{E(E-2B)} \tag{45}$$

and F is the incomplete elliptic integral of first kind

$$F(\varphi,k) = \int_0^{\sin\phi} dx \frac{1}{\sqrt{(1-x^2)(1-k^2x^2)}}$$

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