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Geant4 physics processes for microdosimetry simulation: Very low energy electromagnetic models for protons and heavy ions in silicon

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ABSTRACT

The Geant4-DNA extension of the Geant4 Monte Carlo simulation toolkit aims at modeling early biological damages induced by ionizing radiation at the DNA scale, and it can now track particles down to very low energies in liquid water. New models, called "MuElec", have been implemented for microelectronic applications following the same initial theory, to track low energy electrons in silicon. This paper presents the extension of these MuElec models to incident protons and heavy ions in silicon. First, the theory of the model is presented. The resulting cross sections and stopping powers are compared with data from the literature. The model is then implemented in Geant4 and used to simulate proton tracks. Various physical quantities are extracted from the simulation, and compared with data from the literature and with results from simulation using other Geant4 models. It is shown that the generation of low-energy electrons results in more physically meaningful low-energy secondary electron tracks, which significantly modifies the proton and ion track core on the nanometer scale.

1. Introduction

The simulation of radiation effects in electronic systems is a critical concern in various domains, such as spacecraft missions or for instrumentation in nuclear power plants or medical equipments. With the decrease of size following the technological roadmap [1], accurate prediction of the sensitivity of electronic devices requires more and more detailed descriptions of ionization profiles. The Monte Carlo simulation toolkit Geant4 [2,3] is a suitable tool to address this issue and model the microscopic pattern of energy deposition related to an ionizing particle track structure, involving a detailed modeling of the trajectory of all secondary particles [4,5]. It has already been used successfully, in combination with TCAD simulations [6] or in SEE prediction tools [7,8], to study the sensitivity of advanced electronic devices, down to the 45 nm node. However, inherent limits in Geant4 ionization models prevent its use at smaller scales: the recommended production threshold energy of 250 eV for secondary electrons in the low energy electromagnetic package [9] limits the accuracy of the heavy ion track below 10 nm [6]. In order to study the effect of ionizing particles in future highly scaled integrated circuits by means of simulation, new ionization models are needed, lowering as much as possible this production threshold energy of secondary electrons.

Such models are already implemented in Geant4, but are restricted to water. These developments are part of the Geant4-DNA project, intended for biological applications [10,11]. To be used for microelectronic simulations, they need to be extended to other materials, silicon in particular. Various individual initiatives have been conducted over the years, but no open access version is available for the community. In particular, the work of Akkerman et al. aims at generating and tracking electrons down to an energy of 1.5 eV in silicon [12–15]. It relies on the same theoretical framework as the Geant4-DNA package for the calculation of ionization inelastic cross-sections. The goal of this paper is to use the approach described in [12–15] to calculate these cross-sections and to include them in the open-access frame of Geant4, using the already existing Geant4-DNA classes as a basis for implementation. This approach has already been used to describe electron energy losses in silicon [16,17]. This paper deals with the extension of the model to the generation of low energy electrons by incident protons and heavy ions. To avoid any confusion given the different domains of application, the new models are implemented separately from the Geant4-DNA extension, under the name "MuElec" (for microelectronics).

First, the theory used to calculate the inelastic cross-sections is presented. The main calculation steps are only briefly described, being similar for all incident particles and already extensively detailed in [16,17] for electrons. Various parameters are then calculated from these cross-sections and compared with data from the

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literature to validate the implementation. Finally, resulting proton tracks in silicon simulated with MuElec models are presented. The differences between these tracks and those obtained using the low energy ionization models already available in Geant4 are particularly highlighted.

2. Theory

In Geant4-DNA for water and in the code by Akkerman et al. [12–14] for silicon, the inelastic interaction cross sections σ, are calculated using the complex dielectric function theory [18,19]. All calculations are based on the modeling of the Energy-Loss Function (ELF):

$$ELF(\hbar\omega, \vec{q}) = \mathrm{Im}\left[\frac{-1}{\varepsilon(\omega, \vec{q})}\right]$$

Where $\varepsilon(\omega, \vec{q})$ is the complex dielectric function, with $\hbar\omega$ and $\vec{q}$, respectively, the energy and momentum transfer from the incident particle to an electron of the target material. While the ELF is not easily measured, the Optical Energy-Loss Function (OELF), which is the particular case at $\vec{q} = \vec{0}$ can be deduced from experimental optical data [20,21]:

$$\mathrm{OELF} = \mathrm{ELF}(\hbar\omega, \vec{0}) = \mathrm{Im}\left[\frac{-1}{\varepsilon(\hbar\omega, \vec{0})}\right]$$

This function exhibits a main peak and several discontinuities. The main peak is located at the silicon plasmon energy E_P = 16.7 eV and is attributed to a prominent collective excitation of valence electrons. The discontinuities correspond to shell effects and can be related to ionization energies of the target material electrons.

The experimental OELF is then modeled using an extended-Drude expression [22] similar to the one used by Akkerman et al. [12–15].

$$\mathrm{OELF} = \sum_j D_j(\hbar\omega) \tag{1}$$

Each element of the sum is used to fit one peak of the experimental curve. The function is thus calculated with six peaks whose position is related to energies with physical meaning: the plasmon energy E_p and ionization energies related to the silicon electron configuration $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$: one peak for the K-shell (1s), two for the L-shell (2s and 2p) and two for the M-shell (3s and 3p – making it three with the plasmon peak). The details and validation of this fit are presented in [16,17].

The ELF at $\vec{q} \neq \vec{0}$ is then obtained by introducing a quadratic dispersion relation for the expression of one parameter of the function D_j (see [16,17] for more details).

From the ELF, the Differential Cross-Section (DCS) is calculated for each shell for incident particles of kinetic energy E using equation (2):

$$\frac{d\sigma}{d(\hbar\omega)}(E, \hbar\omega) = \frac{1}{\pi \mathrm{Na}_0 E}\int_{q_-}^{q_+} \mathrm{ELF}(\hbar\omega, \vec{q})\frac{dq}{q} \tag{2}$$

where N is the atomic density of silicon, a_0 the Bohr radius and $q_\pm$ is expressed as: $q_\pm = \frac{\sqrt{2m_e}}{\hbar}(\sqrt{E} \pm \sqrt{E - \hbar\omega})$ for incident electrons, $q_- = \frac{\omega}{v}$ and $q_+ \to \sqrt{2m_e eE_{\max}}/\hbar$ for other incident particles. m_e and e are, respectively, the electron mass and charge, v is the incident particle velocity and E_{max} is the maximal energy transferred to secondary electrons, defined as:

$$E_{\max} = 2m_e c^2 \varepsilon(\varepsilon + 2) \tag{3}$$

with $\varepsilon = E/Mc^2$ for an incident particle of kinetic energy E and mass M.

One DCS is calculated for each of the six peaks used to fit the experimental OELF: in Eq. (2), instead of using the complete expression of the ELF, it is decomposed according to Eq. (1) and one DCS is calculated for each element of the sum, i.e. each of the six peaks of the ELF. To get the DCS for a given shell, the contribution of, respectively, three, two and one peaks are then summed for, respectively, the M-, L- and K-shell. A second integration over the energy transfer $\hbar\omega$ gives the cross-section as a function of the incident particle energy E.

3. Validation and range of applicability of inelastic cross-sections

3.1. Incident protons

For protons, the resulting partial cross-sections, so called "MuElec" cross sections, calculated for each shell are reported in Fig. 1, as a function of the incident particle energy (for the L- and M-shells, two and three peaks of the ELF are summed, respectively). They are compared with results from calculations using the semi-classical Gryzinski's model [23]. For the M-shell, the agreement is good above 50 keV, with less than 20% difference between both cross-sections. This is particularly important since the M-shell is the main contributor in the energy-loss process. Below this energy, large differences occur; this was already observed for incident electrons below 50 eV in [17]. Indeed, the dielectric function theory is a first Born approximation theory, which is known to fail at low incident energy. Higher-order corrections need to be added, that may be considered in future work, i.e. the Barkas-Andersen and Bloch corrections [24]. While these corrections are usually directly applied to the stopping power calculations, adding respectively a Z_{eff}^3- and Z_{eff}^4-correction term to the classical Z_{eff}^2-proportional stopping power formulation, they can be adapted to be used in the differential cross section formulation, as done in [25].

For now, considering the very large differences between this work's cross sections and Gryzinski's calculations below 50 keV, this value will be taken as the lowest limit of validity for this model for incident protons.

For, the L-shell, the measurements performed by Ariyasinghe et al. are also reported [26]. The agreement between all data is reasonable between 50 and 150 keV (less than an order of magnitude

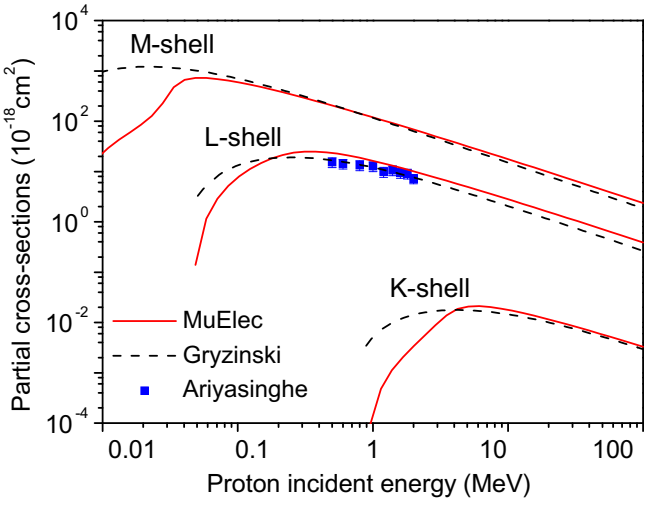

Fig. 1. Calculated proton partial cross-sections compared to the calculations from Gryzinski's classical model [23] and experimental results of Ariyasinghe for the L-shell [26].