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Role of the tail of high-energy secondary electrons in the Monte Carlo evaluation of the fraction of electrons backscattered from polymethylmethacrylate

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ABSTRACT

This work describes a Monte Carlo algorithm which appropriately takes into account the stochastic behavior of electron transport in solids and the simulation of the energy distributions of the secondary and backscattered electrons from polymethylmethacrylate irradiated by an electron beam. The simulation of the backscattered and secondary electron spectra also allows calculating the backscattering coefficient and the secondary electron yield of polymethylmethacrylate as a function of the initial energy of the incident electrons. Results of the simulation are compared with the available experimental data. The importance of considering all the electrons emerging form the surface in calculating the secondary electron yield and the backscattering coefficient is highlighted. In particular, we will discuss the importance of taking into account the tail of high energy secondary electrons in the spectrum for the simulation of the backscattering coefficient.

1. Introduction

The study of the electronic and optical properties of the matter is of great importance for our comprehension of physical and chemical processes which occur in solids. Electronic structure study represents only one example where electron–matter interaction mechanisms play a fundamental role. There are many applicative areas where electron–matter interaction is involved. In particular, let us just mention electron cloud effect on the wall-surface of the particle accelerator vacuum chambers [1–3], electron interaction with the spacecraft surfaces [4–6], nano-metrology for the most advanced CMOS processes [7–9], scanning electron microscopy [10–12], Lorentz microscopy [13–15], and electron spectroscopies [16,17].

Other very important fields which deserve to be mentioned are: plasma processing of materials, local melting of materials for joining large components, plasma-wall in fusion reactors, electron multipliers, electron lithography, and radiation damage. Radiation damage due to electrons interaction with the biological tissues, in particular, is important in the therapies which uses hadron beams. In fact, in proton cancer therapy, we wish to minimize the effects of the irradiation on the healthy tissues near to the diseased cells. When fast protons propagate through organic targets, a large number of secondary electrons are generated, and this process is followed by the subsequent propagation of the secondary electrons in a nanometer scale [18]. Along the track of the incident protons, the shower of secondary electrons is a potential source of radiation damage. Secondary electrons of very low energy are toxic for the human body cells, since they produce damage to the biomolecules due to ionizations/excitations and the resulting break of chemical bonds. Also the secondary electrons with ultra-low energies, which in the past were thought to be relatively harmless, are dangerous for the biomolecules due to the so-called "dissociative electron attachment" [19,20].

This work describes a Monte Carlo algorithm which takes into account the stochastic behavior of electron transport in solids and treats event-by-event all the elastic and inelastic interactions between the incident electrons and the particles of the solid target [21].

It was recently demonstrated that the choice of the optical data model strongly influences the results of a simulation [22]. A comparison of the inelastic mean free paths calculated using extended Mermin [23,24] and extended Drude theory [25] is presented in Ref. [22]. Extended Mermin theory [23,24] was utilized in this work.

The Monte Carlo algorithm was implemented in a computer code in order to simulate the energy distributions of the secondary and backscattered electrons from polymethylmethacrylate

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(PMMA) irradiated by an electron beam. Several values of the initial kinetic energy of the incident electrons are considered, and the evolution of the shape of the spectra is investigated.

The simulation of the backscattered and secondary electron spectra also allows calculating the secondary electron yield and the backscattering coefficient of PMMA as a function of the initial energy of the incident electrons. According to the experimental convention, the secondary electron yield is calculated integrating the spectra of all the emitted electrons in the energy range from 0 to 50 eV. According to the same convention, the backscattering coefficient is calculated integrating the spectra of all the emitted electrons in the energy range from 50 eV to the primary electron energy E_0.

We discuss the effect of ignoring the tail of high energy (>50 eV) secondary electrons in the calculation of the backscattering coefficient and of ignoring the tail of low energy (<50 eV) backscattered electrons in the calculation of the secondary electron yield. Neglecting these tails is quite usual in many Monte Carlo simulations of both secondary electron yields and backscattering coefficient even if it is clear that, since the experiment cannot distinguish between electrons, all the ejected electrons have to be considered in the integration from 0 to 50 eV (calculation of the secondary electron yield) and from 50 eV to the primary energy (calculation of the backscattering coefficient).

We demonstrate, on the one hand, that ignoring the tail of high energy secondary electrons (in the primary energy range from 50 to 1500 eV and for PMMA) introduces errors in the estimation of the backscattering coefficient calculation.

Neglecting the tail of low energy backscattered electrons has, on the other hand, small or negligible effects on the evaluation of the secondary electron yield. These effects are furthermore confined to primary energies smaller than 200 eV.

2. Theoretical framework

The results presented in this paper were obtained using differential and total elastic scattering cross sections calculated utilizing Mott theory [26–28], *i.e.* numerically solving the Dirac equation in a central field; this procedure is known as the "relativistic partial wave expansion method" and it has been demonstrated to provide excellent results when compared to experimental data [29–31]. For details about the present calculations of the Mott cross section, see Ref. [32].

On the side of the energy losses, the inelastic mean free paths are calculated by taking into account the inelastic interactions of the incident electrons with atomic electrons, phonons, and polarons.

The calculation of the electron–electron inelastic scattering processes was performed within the Mermin theory [23]. The Mermin dielectric function is given by

$$\varepsilon_M(\boldsymbol{q},\omega) = 1 + \frac{(1+i/\omega\tau)[\varepsilon^0(\boldsymbol{q},\omega+i/\tau)-1]}{1+(i/\omega\tau)[\varepsilon^0(\boldsymbol{q},\omega+i/\tau)-1]/[\varepsilon^0(\boldsymbol{q},0)-1]}, \quad (1)$$

where $\boldsymbol{q}$ is the momentum, ω the frequency, τ the relaxation time, and $\varepsilon^0(\boldsymbol{q},\omega)$ the Lindhard dielectric constant [33].

Indicating with e the electron charge, $f_{\boldsymbol{p}}$ the Fermi–Dirac distribution, and $\varepsilon_{\boldsymbol{p}}$ the free electron energy, the Lindhard dielectric constant $\varepsilon^0(\boldsymbol{q},\omega)$ is given by

$$\varepsilon^0(\boldsymbol{q},\omega) = 1 + \frac{4\pi e^2}{q^2} B(\boldsymbol{q},\omega), \quad (2)$$

$$B(\boldsymbol{q},\omega) = \int \frac{d\boldsymbol{p}}{4\pi^3} \frac{f_{p+q/2} - f_{p-q/2}}{\omega - (\varepsilon_{p+q/2} - \varepsilon_{p-q/2})/\hbar}. \quad (3)$$

If we now consider a superposition of free and bound oscillators, for any oscillator the energy loss function (ELF) is the opposite of the imaginary part of the inverse of the Mermin dielectric function. It is given by

$$Im\left[\frac{-1}{\varepsilon_M(\omega_i,\gamma_i;\boldsymbol{q},\omega)}\right] = \frac{\varepsilon_{M_2}}{\varepsilon_{M_1}^2 + \varepsilon_{M_2}^2}. \quad (4)$$

where

$$\varepsilon_M = \varepsilon_{M_1} + i\varepsilon_{M_2} \quad (5)$$

and ω_i, and γ_i are, respectively, the frequency and the damping constant associated to any oscillator.

According to Abril et al. [24], a linear combination of Mermin-type energy loss functions, one per oscillator, allows to calculate the electron ELF, for $q = 0$, for any given material:

$$Im\left[\frac{-1}{\varepsilon(q=0,\omega)}\right] = \sum_i A_i Im\left[\frac{-1}{\varepsilon_M(\omega_i,\gamma_i;q=0,\omega)}\right]. \quad (6)$$

A_i, ω_i, and γ_i are determined looking for the best fit of the available experimental optical ELF.

The Ritsko et al. experimental optical data [34] were used for evaluating the parameters A_i, ω_i, and γ_i of PMMA: the value of these parameters were calculated and reported by de Vera et al. and can be found in Ref. [35].

Once obtained the parameters corresponding to the best fit of experimental optical data, ELF($q = 0$), the extension out of the optical domain ($q \neq 0$) can be obtained by [24]

$$Im\left[\frac{-1}{\varepsilon(q,\omega)}\right] = \sum_i A_i Im\left[\frac{-1}{\varepsilon_M(\omega_i,\gamma_i;q,\omega)}\right]. \quad (7)$$

Note that the dispersion law is included in the Mermin theory, and it is not necessary, as in the case of the Drude–Lorentz approach, to introduce an approximate expression of it to extend the ELF beyond the optical domain.

Knowledge of the energy loss function allows calculating the differential inverse inelastic mean free path (DIIMFP), given by

$$\frac{d\lambda_e^{-1}}{d\hbar\omega} = \frac{1}{\pi a_0 T}\int_{q_-}^{q_+}\frac{dq}{q} Im\left[\frac{-1}{\varepsilon(q,\omega)}\right], \quad (8)$$

where a_0 is the Bohr radius, E is the kinetic energy of the incident electrons and

$$q_\pm = \sqrt{\frac{2m}{\hbar^2}}(\sqrt{E} \pm \sqrt{E-\hbar\omega}). \quad (9)$$

The Mermin DIIMFP of electrons in PMMA is represented in Fig. 1, for kinetic energies of the incident electrons in the range from 50 to 1000 eV.

The inverse of the integral of every curve presented in Fig. 1 provides, for each kinetic energy E, the inelastic mean free path λ_e. For a discussion about PMMA inelastic mean free path calculation using different approaches, see Refs. [22,36].

Other mechanisms of inelastic scattering and energy loss are related to the electron–phonon and to the polaronic effect. Electron–phonon interactions were described using the Fröhlich theory [37,38]. Polaronic effect was modeled according to the law proposed by Ganachaud and Mokrani [39]. The introduction of these effects is important because, when the electron energy E becomes lower than ~20–50 eV, the dielectric formalism presented so far is no longer able to accurately describe energy loss phenomena. In this region, electrons lose energy in many small amounts interacting with phonons, in particular with the optical modes of lattice vibrations. In his theory of the electron–phonon interaction, Fröhlich [37] described the interaction of free conduction electrons with the longitudinal optical mode lattice vibrations. Since, according to Ganachaud and Mokrani [39], the dispersion relation of the longitudinal phonons can be neglected in the optical branch, one can use a single phonon frequency ω. Using Fröhlich

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