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Delta-electron spectra, inelastic cross sections, and stopping powers of ions in silicon: Comparison between different models

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ABSTRACT

The energy spectrum of the δ-electrons ejected by an ion moving in the bulk of a solid is the origin of numerous effects which follow the transport of these electrons. This spectrum cannot be measured directly. Therefore, it should be derived theoretically. The present work aims to investigate the uncertainties introduced when applying commonly used theoretical approaches like BEA, CDFT, and PWBA to calculate δ-electron spectrum. Our calculations show that, above a certain δ-electron energy, the energy spectra of the δ-electrons obtained using the various approaches behave similarly. Below this energy, the spectra found using these approaches differ significantly due to the manner in which the solid state character of the target material is taken into account in each approach. This results in differences in the inelastic cross sections and stopping powers for the ions, which in turn result in different ion track structures. Also discussed in this paper is the effect of the uncertainty in the effective ion charge on the accuracy of ion track calculations. The results obtained for silicon allow estimating the possible uncertainties of the calculated ion track properties and related effects.

1. Introduction

The study of swift ion tracks in matter and their effects is a significant and a developing area of activity in physics of high-density energy deposition in solids, radiobiology, semiconductor technology, and other applications [1]. We meet here a sequence of processes (often overlapping), starting from instantaneous (during less than 1 fs) energy delivery to the atomic system of the solid within a nanometric range from the track axis, through a transition process (lasting up to few picoseconds) of redistribution of the transferred energy to the target electrons in a more extended region (up to few micrometers), to the final stage of creating measurable changes of the properties of the matter. As shown in the review article of Rothard [2], only few experimental methods are available for measuring the first and second stages of the above processes.

The primary physical process ("the precursor") of initialization of ion-induced tracks in matter and of the resulting track effects is the ejection of δ-electrons from the target atoms by the swift ions. These electrons are characterized by an energy spectrum. A review on the status of experimental and theoretical study of spectra of electrons ejected from single atoms and molecules was given by Rudd et al. [3].

The information on the evolution of the transient phases of track formation, which start with the δ-electron ejection, can be obtained from calculations based on physical models of the interaction of the ejected electrons with matter. The realization of such calculations is a complicated task due to different origins of the transient processes (such as Auger recombination, cascade of ionizations, energy transfer to phonons, etc.), which accompany the primary process in solid matter. Moreover, there are no verified theories for them. Nevertheless, after some simplifications, calculations of track formation may be done by computer simulations using various methods, including molecular dynamics (MD) and Monte Carlo (MC).

The widespread detailed MC algorithm for charged particle transport in matter uses two basic steps: (i) determining the type of the interaction (i.e. elastic, inelastic, bremsstrahlung, etc.), for which one needs the data on the relative probabilities of all the possible interactions which are calculated from the corresponding cross sections (the nuclear interactions will be ignored here), and (ii) sampling from the differential distributions of energy transfer to the δ-electrons (ejected by the ion) or of secondary electrons (ejected by the δ-electrons) in the randomly selected interaction process in the previous step. Fortunately, the transport calculations of electrons in matter by MC methods are precise enough and their results agree quite well with the experimental data (see [4–6] and references therein).

In this paper, we focus on the *primary* process of δ-electron ejection in silicon by protons and heavy ions and compare the energy spectra of these electrons calculated using different approaches: the classical binary encounter approximation (BEA) [7–9], the

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complex dielectric function theory (CDFT) [10–12], and the results of quantum mechanical calculations using the plane wave Born approximations (PWBA) [13,14]. Recently, the spectrum of the δ-electrons ejected by swift ions was examined in [15], based on two different models of excitation of the electronic system of the atoms in SiO_2. It was shown that difference in the resulting spectra can be seen only at the high-energy region, which may affect the lateral periphery of the ion track.

The aim of the present investigation is to understand what uncertainties in the track structure and the track effects in silicon are introduced using these approaches. We will also compare the *K*-, *L*-, and *M*-shell ionization cross sections and the stopping powers calculated on the basis of these approaches. Then, we will discuss how the different approaches affect the radial distribution of the deposited energy – a key parameter to characterize the single event upset (SEU) phenomenon [16] in silicon-based electronic devices [17–19]. The spectra of electrons ejected by protons and heavier ions considered in our work do not take into account the changes in the electronic system of the *projectile* moving in the solid and the different wake effects, which are described in [2] but which are still not completely understood. To a certain extent, these effects are expressed in Z_{eff} – the effective charge of the ion used as the scaling parameter to calculate the differential and total inelastic ion–electron interaction cross sections and the stopping power from the corresponding proton (or α-particle) data. We will discuss the expressions used in calculating Z_{eff} and their effects on ion track characteristics.

2. δ-Electron energy spectra

2.1. Differential cross sections for proton ionization of silicon

One of the first theoretical expressions (obtained using a simplified version of the BEA) for the energy spectrum of δ-electrons ejected in the collision of an ion with the target-atom electrons was proposed by Bradt and Peters [20]. The differential cross section that an ion with energy E_{i} (in MeV/amu) and effective charge Z_{eff} transfers energy E to the ejected electron from the n shell is given by:

$$\frac{d\sigma}{dE}=\frac{2\pi e^4 Z_{\mathrm{t}} Z_{\mathrm{eff}}^2}{m_0 c^2 \beta^2 E^2}\left[1-\frac{\beta^2 E}{E_{\max}}+\frac{\pi\beta Z_{\mathrm{eff}}^2}{137}\left(\frac{E}{E_{\max}}\right)^{1/2}\left(1-\frac{E}{E_{\max}}\right)\right]. \tag{1}$$

We note in passing that we will use throughout the paper the terms "differential cross section" and "energy spectrum" interchangeably, as these two are proportional, with the proportionality constant given by the integral of the former over the ejected electron energy. Here β is the ion velocity v in units of light velocity, $\beta = v/c$, whose value is given by $\beta^2 = E_{\mathrm{i}}(E_{\mathrm{i}}+1876)/(E_{\mathrm{i}}+938)^2$, m_0 is the electron mass, Z_{t} is the target atom nuclear charge, and $E_{\max}$ is the maximal energy transferred to the δ-electron in an ion–electron collision. In Eqs. (1)–(3) below, the energy transfer E is equal to the sum of kinetic energy imparted to the electron E_δ and its binding energy E_{bn} in the n-shell, $E = E_\delta + E_{\mathrm{bn}}$. Similarly, $E_{\max} = E_{\delta\max} + E_{\mathrm{bn}}$, where $E_{\delta\max}$ is the maximal kinetic energy of the ejected electron, $E_{\delta\max} = 2m_0c^2\beta^2(1-\beta^2)^{-1}$. The transformation from $d\sigma/dE$ to $d\sigma/dE_\delta$ is evident. For protons, we assume $Z_{\mathrm{eff}} = 1$, irrespective of their energy. This is valid for energies $E_{\mathrm{i}} \geqslant 1$ MeV, considered in this work. For heavier ions, the values of Z_{eff} to be used in Eqs. (1)–(3) will be discussed in Section 4.

Eq. (1) was successfully used by Katz et al. [21] for analytical calculations of the radial distribution of the energy deposited by swift ions in water and tissue equivalent materials.

Geant4 code [22] uses a simplified version of Eq. (1) for the same spectrum:

$$\frac{d\sigma}{dE}=\frac{2\pi r_0^2 m_0 c^2 Z_{\mathrm{t}} Z_{\mathrm{eff}}^2}{\beta^2 E^2}\left[1-\frac{\beta^2 E}{E_{\max}}+\frac{E^2}{2E_{\max}^2}\right], \tag{2}$$

where r_0 is the classical electron radius. The last term in Eq. (2) is for particles with spin ½.

Both spectra behave similarly as function of transferred energy E (see Fig. 1 below). The advantage of Eq. (2) is that it enables having a simple algorithm for energy transfer sampling in MC simulations [22]. The ejected electron in both formulas is assumed to be initially at rest.

The angular distribution of the ejected electrons $d\sigma/d\theta$ (θ is the angle between the direction of the incident ion and that of the emitted δ-electron) is treated as independent of the energy loss spectrum. The angle θ is given by $\theta = \cos^{-1}(E_\delta/E_{\delta\max})^{1/2}$. Unless E_δ is close to $E_{\delta\max}$, $\theta \approx \pi/2$. The angular distribution is thus almost a δ-function around $\pi/2$. For track creation in the bulk of the material, we used a more elaborate expression for the distribution of the angle θ. However, this should practically not influence the radial distribution due to the very quick randomization of the electron-direction through elastic and inelastic scatterings. The exact angular distribution becomes important when considering δ-electron emission from very thin films [2,3].

The spectrum of the energy transferred from the ion to the target electrons can also be calculated using the *two-particle classical Coulomb collision* theory. This is also a BEA theory but it includes the velocity distribution of target-atom electrons according to the formulas proposed by Gryzinski [7] for protons. It was later improved by Garcia [8] and recently by Kaganovich et al. [9 and references therein]. Due to their cumbersome form, we will not present them here.

The CDFT (which is a first-order Born approximation theory) was used in many studies, starting from the pioneering works [10,11], which calculated the interaction cross section of charged particles with the electronic subsystem of the solid, and continuing with MC codes for practical cases like track structure and SEU in silicon devices [19].

The CDFT cross section for energy transfer is given by [23]:

$$\frac{d\sigma}{dE}=\frac{2Z_{\mathrm{eff}}^2 e^2}{\pi N\hbar^2 v^2}\int_{q^-}^{q^+}\frac{1}{q}\mathrm{Im}\left[\frac{-1}{\varepsilon(\omega,q)}\right]dq, \tag{3}$$

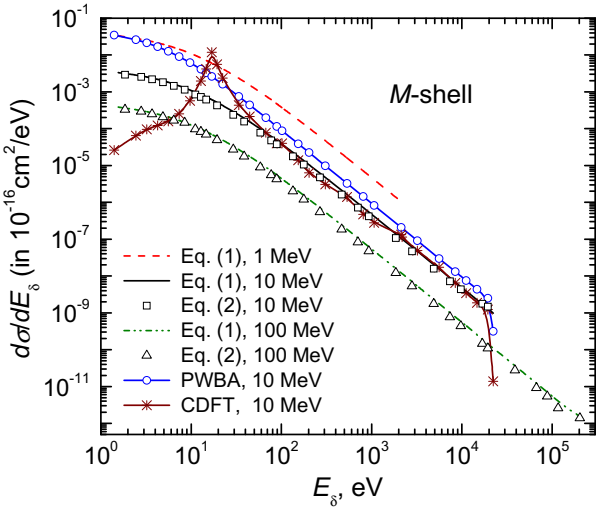

Fig. 1. Comparison between the results of Eqs. (1) and (2) (Geant4 formulation), Eq. (4) (PWBA), and Eq. (3) (CDFT) for the spectra of δ-electrons ejected by protons from the silicon *M*-shell. Dashed, solid and dotted lines are the results of Eq. (1) for protons with energies of 1, 10, and 100 MeV respectively. The symbols are the results of Eq. (2) for protons with energies of 10 and 100 MeV. Lines with symbols are the PWBA and CDFT results for 10 MeV protons.