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Transport of electrons and positrons impinging on solid targets: A comparative study performed by using a Monte Carlo simulation

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ABSTRACT

Using the Monte Carlo simulation technique, the behaviour of electrons and positrons when impinging on solid targets has been investigated. The examined particle energy range is 1–5 keV. For that purpose the elastic scattering is based on exact cross sections of effective crystalline potentials whereas inelastic scattering processes are described by the Penn model and Ashley theory for positrons and electrons, respectively. The obtained results for aluminium, silver and gold semi-infinite targets are compared with the available experimental and theoretical data reported in the literature. Very good agreement is observed between our findings and experiment. The differences and the similarities between positrons and electrons penetration and backscattering features have been examined and discussed.

1. Introduction

In the last decade there has been a resurgence of interest in the use of charged particles as a probe for investigating a wide variety of systems [1,2]. The continuing progress in the development of intense monochromatic beams of low energy electrons and positrons has made it possible to perform a number of land mark experiments. The low energy electrons impinging on solid targets are of great interest in electron spectroscopy and microscopy and electron microlithography [1,3,4]. In addition, the use of low voltage scanning electron microscopy is of particular importance in the examination of semiconductors as well as in biology and metrology [5,6]. On the other hand, positron beams have led to a whole new class of possible experiments when directed at a solid surface. Indeed, low-energy positron beams may be seen as the antimatter complement to electron beams commonly used in many diagnostic probes and other useful devices. In fact, while useful information on electronic structures in solid materials were obtained from positron annihilation techniques [7–11], low-energy beams of positrons may allow the knowledge of defect profiling near surfaces and provide important information about the nature and the distribution of point defects in solids [12–18]. Although there is considerable interest in the study of surfaces using electrons and positrons as probes, the understanding of the behaviour of low-energy electrons and positrons (in the keV and sub keV range) remains unsatisfactory for both theory and experiment.

The better understanding of the electron beam interactions at low energies requires the test of certain key measurements against theoretical predictions [6]. The backscattering coefficient of electrons and positrons is one of the key measurements, since it can be both relatively easily measured experimentally and calculated theoretically. Backscattered electrons or positrons refer to those charged particles which are, when directed towards a solid target at some incident energy, scattered and returned into the vacuum. In terms of theoretical investigations, the accuracy of the backscattering coefficient depends on the accurate modelling of the interactions of the charged particles with the sample under study [1,19–25]. Once the scattering processes are described, the behaviour of charged particles in the materials of interest can be studied by the use of the Monte Carlo simulation, a numerical procedure often used to solve mathematical problems involving the interactions of very large numbers of particles [1,18,26–29]. The method has been proved to be very successful in modelling individual charged particle trajectories resulting from a series of random scattering events as random walks.

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In the present contribution, a Monte Carlo simulation of electron and positron slowing down in semi-infinite Al, Ag and Au has been performed. The aim of this work is to compare the behaviour of electron and positron when impinging on these metals in order to investigate the differences and the similarities. In this respect, the electron and positron inelastic mean free paths, penetration depths and backscattering coefficients in Al, Ag and Au materials have been calculated as a function of the primary energy of the incident particles. The accuracy of the Monte Carlo method depends crucially on the modelling of the scattering processes employed in the simulations. To model elastic scattering, Valkealahti and Nieminen [30] have used the Rutherford differential cross section, modified to account for electronic screening. However, their results showed that the screened Rutherford cross section is not accurate for scattering off atoms at energies in the range of 1–10 keV. To overcome this shortcoming, we have previously modelled the elastic scattering using a modified Rutherford differential cross section in which the numerical coefficient in the atomic screening parameter is taken to be dependent of the particle incident energy [14,31]. Although this approximation has improved the results regarding the backscattering coefficients, it requires a fit of the cross section to that from partial wave expansion method for each energy and material under load. Furthermore, one needs to make an interpolation for determining the dependence of the numerical coefficient on the particle energy. This is a complicated task and requires available data in the literature. In order to avoid all these complications, in the present paper the elastic scattering cross sections for both electrons and positrons have been obtained from a partial wave expansion [32]. The same method with some differences in details has been previously used by Dapor [22], Jensen and Walker [21] and Bouarissa and Walker [33] and appeared to work well. To model inelastic scattering, Gryzinski [34] and Salvat et al. [35] have used simple semi-empirical atomic cross sections which worked well at energies higher than about 5 keV. However these expressions failed to describe scattering off valence electrons, which dominates at low energies. Many researchers have handled inelastic processes in terms of Gryzinski's excitation function expressions [30,31,36,37] but incorporated some modifications with valence electrons and examined alternatives to the core electron scattering cross sections [20]. Dapor [38] has computed the energy loss by using the Kanaya and Okayama [39] semi-empirical expression. For simple metals, valence electron scattering can be described using the dielectric scattering formalism [40]. This is not the case for non-simple metals where more detailed descriptions of the valence electron scattering cross sections are needed. Shimizu and Ding [41] have used a simplified version of the Penn model in electron simulations. Jensen and Walker [21] have used for the first time the full Penn model for inelastic scattering in a Monte Carlo simulation of the penetration of positrons and electrons through solids. Their results showed that the agreement with experiment is less good for electrons than for positrons. This discrepancy has been accounted for by the neglect of indistinguishibiliy of electrons in the Penn model. In our previous work and in order to model inelastic cross sections, we have used modified Gryzinski's cross sections [14,31,33]. In the present paper, the inelastic scattering cross sections for positrons are described using the Penn dielectric loss function [42], whereas in the case of electrons, the inelastic scattering processes were handled using the Ashley theory [43]. The present Monte Carlo programme has the same general structure as that used by Jensen and Walker [21] but we have incorporated more realistic inelastic scattering cross sections in the case of electrons. We compare our simulation results with backscattering measurements which provide stringent tests on the accuracy of the description of the scattering processes in the simulations.

2. Method of calculation

The elastic scattering is described by the scattering of a plane wave representing the electron or positron off an atomic electrostatic potential due to the nucleus and electrons in the atom. The scattering potential is constructed by a superposition of free-atom potentials representing an atom embedded in a crystal. The free-atom electrostatic potentials are obtained from a density functional calculation using the local-spin-density approximation [44].

The differential cross section is calculated from the partial wave expansion [32]. Each phase shift is obtained from a numerical solution of the radial Schrödinger equation for angular momentum quantum number l. Further details about the scattering potential and the determination of the phase shifts are given in Refs. [20,33]. At each energy sufficient l-values are included so as to give a relative error in the differential cross sections of less than 10^{-2}.

The inelastic scattering cross sections for positrons are obtained using the Penn model [42]. The model is found to be accurate for positrons [21], but it overestimated stopping powers and underestimated mean free paths for electrons. Furthermore, at low energies, the assumption that the incident particles have a free-particle band structure in the Penn model, is a reasonable approximation for positrons at all energies [21,45], but it breaks down at low energies for electrons in most solids. Thus, in the case of electrons, the inelastic scattering processes are handled in terms of the Ashley theory [43]. The latter relies on experimental optical data for the construction of the dielectric loss function, similarly to the Penn model, but is sufficiently simple that the indistinguishability between electrons and positrons can be taken into account.

3. Simulation procedure

In the present contribution, the calculation are performed for a semi-infinite Al, Ag and Au targets with a planar surface. The normal incidence of the initial electrons and positrons is assumed. In most cases 10^4 incident particles are simulated in each simulation run. The trajectory of each particle is followed until either the energy of the charged particle is less than a cut-off energy (20 eV in the present work, counted as implanted particle) or until it has left the solid (counted as backscattered particle). The simulation employs random numbers all of which are taken from uniform distribution between 0 and 1. The total scattering cross section determines the mean free paths of the electrons or positrons. The distance travelled between collisions is chosen by a random number. Another random number selects which type of scattering takes place. Depending on this type of scattering, either one or two random numbers then determine the angle of scattering and/or the energy loss. The scattering angle is determined in the particle frame of reference. We then transform the scattering angle back into the sample frame of reference, and calculate the position of the particle. A spherical polar coordinate system is used for all the scattering calculations. In this system the z-axis is normal to the sample surface. The azimuthal angle is taken from the x-axis to the projection of the velocity vector of the particle onto the xy plane. In an isotropic medium this angle is randomly distributed between 0 and 2π.

4. Results and discussion

Figs. 1 and 2 display the inelastic mean free paths for electrons and positrons, respectively for the materials of interest. Note that there is a difference between inelastic mean free paths of electrons and positrons where it appears that they are somewhat larger for positrons.