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Electron backscattering from solid targets: Elastic scattering calculations

M. Hannachi [a], Z. Rouabah [a], C. Champion [b], N. Bouarissa [c,*]

[a] Materials and Electronic Systems Laboratory (LMSE), University of Bordj Bou Arreridj, Algeria
[b] Université Bordeaux 1, CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux-Gradignan, CENBG, France
[c] Laboratory of Materials Physics and Its Applications, University of M'sila, 28000 M'sila, Algeria

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ABSTRACT

Analytical expression of the target atomic number dependence of the numerical coefficient in the Nigam atomic screening factor is proposed here to approximate the Rutherford elastic scattering cross sections for slow electron beams impinging on selected solid targets (from Be to Au) in the primary energy range 1–4 keV. Applications are then proposed in terms of Monte Carlo calculation of backscattering coefficient. In this respect, tabulations of backscattering coefficients are here reported for slow electrons in solid targets of interest pointing out a reasonable agreement with the data available in the literature. Analytical expressions of the target atomic number dependence of the electron backscattering coefficient is also suggested for selected electron primary energies ranging from 1 to 4 keV allowing thus an accurate determination of backscattering coefficients for low-energy electrons in solid targets without any resort in Monte Carlo type calculations.

1. Introduction

Interactions of low-energy electron beams with solid targets are of interest in many areas of surface science, solid-state physics and microelectronics [1–3]. Indeed, when a slow electron impinges on a sample, it penetrates the surface and undergoes complicated scattering processes. This penetration is associated with various phenomena which are used to characterize the sample in modern analytical techniques such as electron probe microanalysis, scanning electron microscopy, analytical electron microscopy, Auger electron spectroscopy and electron beam lithography [1].

Backscattered electrons from solid targets play a fundamental role in scanning electron microscopy, electron probe microanalysis, Auger electron spectroscopy, electron beam lithography and radiobiology [1–3]. Hence, their determination became the subject of numerous works [4–11]. In fact, the problem of interactions in solid targets under electron beam bombardment should be able to be solved experimentally by measuring the resulting physical quantities of basic importance [1]. Experimentally, the information lies in the fully differential distributions (in angle and energy) of the backscattered electrons [7]. However, the electron–solid interaction process remains unknown mostly due to the limitation of the current experimental techniques. In this context, a theoretical support remains crucial to extract accurate information in particular when the latter are experimentally unattainable.

The most powerful theoretical technique to study the slowing-down of charged particles in matter is undoubtedly the Monte Carlo tool, which is able to simulate in details the charged particle track structure [1–6,12–18]. The aim of Monte Carlo modelling of electron–solid interactions is, therefore, to simulate these scattering processes as precisely as possible by numerical methods which, as a matter of course, depend on the knowledge of the fundamental mechanisms involved in the slowing-down of the charged particle [1]. Thus, the accuracy of Monte Carlo method crucially depends on the modelling of the scattering processes employed in the simulation, which in turn depend on the electron energy: the dominant processes are elastic scattering of individual atoms and inelastic scattering involving core and valence electron excitations. Thus, Monte Carlo simulation can be used not only to support the interpretation of electron surface experiments but also to provide a convenient way of comparison between theory and experiment.

The current contribution is undertaken so as to focus on slow electrons penetration in a number of selected atomic targets ranging from Be to Au and for impact energies ranging from 1 to 4 keV. The aim of this work is the modelling of elastic scattering cross

* Corresponding author at: Department of Physics, Faculty of Science, University of M'sila, 28000, M'sila, Algeria. Tel.: +213 552624855.
E-mail address: n_bouarissa@yahoo.fr (N. Bouarissa).

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sections via a modified Rutherford approach in which the numerical coefficient in the Nigam atomic screening factor is considered as dependent of the atomic number of the targets. This has been made by using the analytical approximation of the differential elastic scattering cross section as independently developed by Baro et al. [19,20] and by Miotello and Dapor [21] that was used to expedite the calculations in applications such as Monte Carlo simulation. The transport elastic scattering cross sections are obtained using the accurate transport cross sections determined via Rouabah et al. approximation [9]. To model inelastic core and valence electron excitation, the Gryzinski's expressions [22–24] have been used. As an application, the electron backscattering coefficient has been calculated for electrons impinging on a large set of targets of interest. Generally speaking, the obtained results accord with success with the experiment. Furthermore, a numerical coefficient in the Nigam atomic screening factor that depends on the target atomic number has been proposed for all targets of interest. Besides, analytical expressions of the target atomic number dependence of the electron backscattering coefficient regarding all materials under load have been tentatively proposed for given electron primary energies in the range 1–4 keV. Details of the model and promising results are presented.

2. Theoretical details

Valkealahti and Nieminen [12] have modelled the elastic scattering using the Rutherford differential cross section, modified to account the electronic screening, namely

$$\frac{d\sigma_{el}}{d\Omega} = \frac{e^4 z^2}{4E^2(1-\cos\theta+2\beta_N)^2} \tag{1}$$

where z, θ, e, and E are the atomic number, the scattering angle, the electron charge, and the electron energy (in eV), respectively. β_N is an atomic screening parameter given by Adesida et al. [25] as,

$$\beta_N = \frac{2.61 z^{2/3}}{E} \tag{2}$$

The numerical coefficient 2.61 was obtained by taking the best fit of the cross section derived from Rutherford's expression to that from the partial wave expansion method for aluminium.

Using Eqs. (1) and (2), Valkealahti and Nieminen [12] found that the screened Rutherford cross section was not accurate for scattering on atoms at energies in the range of 1–10 keV and gave backscattering coefficients in strong disagreement with experiment. Recently, Bouarissa et al. [26] traced back the non-accuracy of the screened Rutherford cross section to the numerical coefficient which was taken to be constant. To overcome this shortcoming, they took numerical coefficient as a variable depending on the charged particle energy before each collision. Although the idea of Bouarissa et al. [26] led to improved elastic cross sections and hence to accurate backscattering coefficients, the numerical coefficient should be determined for each element under consideration. This is a difficult task since one needs to find a best fit of the total elastic scattering cross section derived from Rutherford's expression to that from the phase shifts for each target element of interest.

In the present work, the numerical coefficient in the Nigam atomic screening factor referred to as μ is taken to be dependent on the target atomic number (z) of several selected solid targets ranging from Be (z = 4) to Au (z = 79) according to the expression:

$$\mu(z) = -1\times10^{-5}z^3 + 2\times10^{-3}z^2 - 5.5\times10^{-2}z + 2.733 \tag{3}$$

Eq. (3) has been obtained by taking the best fit of the total elastic scattering cross section derived from Rutherford's expression to that from the analytical approximation as independently developed by Baro et al. [19,20] and by Miotello and Dapor [21] in the electron energy range of 1–4 keV for all elements of interest.

The analytical approximation of the differential elastic scattering cross section as independently developed by Baro et al. [19,20] and by Miotello and Dapor [21] is

$$\sigma_{tot} = \frac{\sigma_{tr}}{\Gamma\left[\frac{\Gamma+2}{2}\ln\left(\frac{\Gamma+2}{\Gamma}\right)-1\right]} \tag{4}$$

where

$$\Gamma = \frac{me^4\pi^2 z^{2/3}}{h^2 E} \tag{5}$$

In Eq. (4), σ_{tr} is the transport cross-section which was determined for each target element under load by using the accurate transport cross-sections calculated via Rouabah et al. approximation [9].

Inelastic processes have been treated using Gryzinski excitation function expressions [22–24]. To calculate the total inelastic scattering cross section, we have followed the procedure of Bouarissa described in Ref. [27]. At each inelastic scattering event, the energy loss ΔE is calculated by selecting a uniform random number R ($0 \le R \le 1$) and then finding a value of ΔE that satisfies

$$R = \int_{\Delta E}^{E} \frac{d\sigma(\Delta E')}{d\Delta E'} \times \frac{d\Delta E'}{d\sigma_{inel}} \tag{6}$$

This integral is given by the approximate expression: if $\Delta E \ge E_B$ (binding energy),

$$\int_{\Delta E}^{E} \frac{d\sigma(\Delta E')}{d\Delta E'} d\Delta E' = \left(\frac{\pi N_s e^4}{E\times E_B}\right)\left(\frac{E}{E+E_B}\right)^{1.5}\left(1-\frac{\Delta E}{E}\right)^{[1+(E_B/(E_B+\Delta E))]} \times\left\{\frac{\Delta E}{E_B}+\frac{2}{3}\left(1-\frac{\Delta E}{E}\right)\ln\left[2.7+\left(\frac{E-\Delta E}{E_B}\right)^{0.5}\right]\right\}\frac{E_B^2}{\Delta E^2} \tag{7}$$

where N_s is the number of electrons in a particular "shell" contributing to the inelastic events. This expression was used for the first time by Bouarissa [27] and its use has considerably speeded up the simulation. When the random number selection gives a smaller energy loss than the binding energy E_B, the actual energy loss is set to be zero. Eventually, it comes the time when the electron primary energy will be less than E_B; in this case the total inelastic scattering cross section is set to be zero provided that the electron is not backscattered.

3. Simulation procedure

The Monte Carlo simulation of electron transport is based on a stochastic description of the scattering process. The simulation employs random numbers, all of which are taken from uniform distribution between 0 and 1. When an electron impinges on a solid surface it penetrates the solid, undergoing a complicated scattering process. This electron penetration is approximated by a classical zigzag trajectory. In Monte Carlo process, one chooses as a random basis, the type of collision and deflection angle and then moves the electron until the next collision a distance determined by the total scattering cross section. All the scattering calculations are carried out in a spherical polar coordinate system, where the Z axis is normal to the sample surface and normal to it, the angle θ is taken from the Z axis, and the angle φ is taken from the X axis to the projection of the velocity vector of the particle onto XY plane and was evaluated from a uniform distribution.

The Monte Carlo simulation repeats a basic series of steps for each electron trajectory. The trajectory of each electron was followed until it either came back to the surface (backscattered) or slowed down below 20 eV (implanted). All results presented here were obtained for semi-infinite medium with a planar surface with normal incidence of the electrons. Normally 10^4–3×10^4 particle trajectories were calculated in each simulation for each system.