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# Monte Carlo simulation of slow electrons impinging on metals

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**Abstract**

A Monte Carlo simulation technique is used to investigate slow electrons penetration in semi-infinite aluminium and gold in the energy range of 500–4000 eV. Elastic scattering is based on a modified Rutherford differential cross section where the numerical coefficient in the atomic screening parameter is taken to be variable. To model inelastic core and valence electron excitation, we have used the Gryzinski's expression. Our simulated results are compared with the experimental backscattering data and good agreement is observed which suggests that both the transport model and the scattering cross sections used in the present work are reliable. 

The transport of slow electrons in solid targets is very important in electron microscopy, surface electron spectroscopy, electron microlithography and electron-probe microanalysis. All techniques using slow electrons as the primary beam striking a target require an understanding of the processes by which electron slow down in the sample of interest. This has motivated a large body of work on studies of the fundamental aspects of slow electron transport in solids [1–5]. Although there is no complete analytical theory of electron transport in solids, many numerical methods based on the Monte Carlo simulation have been very successful in modeling individual electron trajectories resulting from a series of random scattering events as random walks and simulated in the computer [6–9]. Both the Monte Carlo simulation and the analytical methods require an accurate knowledge of the elastic and inelastic scattering processes suffered by the electrons travelling in the solid target.

Although it is in some cases sufficient to treat inelastic scattering of charged particles in a continuous slowing down approximation [10], the most accurate Monte Carlo method describes both elastic and inelastic scattering as discrete events. To model elastic scattering, Valkealahti and Nieminen [1] have used the Rutherford differential cross section, modified to account for electronic screening,

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

where $z$, $\theta$, $e$ and $E$ are the atomic number, the scattering angle, the electron charge, and the electron energy in eV, respectively. The parameter $\beta_N$ represents an atomic screening parameter which is given by Adesida

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et al. [11] as

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

where the numerical coefficient 2.61 gives the best fit of the cross section derived from Rutherford's expression to that from the partial wave expansion method for aluminum. Unfortunately, the obtained results of Valkealahti and Nieminen [1,2] showed that the screened Rutherford cross section is not accurate for scattering off atoms at energies in the range of 1000–10000 eV and hence its use for modeling elastic scattering leads to poor results for the backscattering probability. In studying slow positron penetration in Al, Bouarissa et al. [10] have shown recently that the reason for non-accuracy of the screened Rutherford cross section lies in the fact that the numerical coefficient (2.61) is taken to be constant, since its value gives the best fit of the cross section derived from Rutherford's expression to that from the partial wave expansion method only for a given energy, whereas the value of the incident charged particle energy decreases gradually once the particle is injected into the material, so before each collision we have a new value of the energy for the particle and therefore we need a new value for the numerical coefficient which gives the best fit for that new energy. We have followed the idea of Bouarissa et al. for electrons and assumed that the value of the numerical coefficient is not constant, but it depends on that of the electron energy before each collision. A best fit of the total elastic scattering cross section derived from Rutherford's expression to that from the phase shifts [3] in the energy range of 500–4000 eV gives

$$\mu(E) = 2.86 \times 10^{-8} E^2 - 1.33 \times 10^{-3} E + 18.4 \tag{3}$$

and

$$\beta_N = \left(0.48 + 1.132 \times 10^{-4} E\right)\left(\frac{\mu z^{2/3}}{E}\right) \quad \text{(for Al)}, \tag{4a}$$

$$\beta_N = \left(1 + 6.41 \times 10^{-4} E\right)\left(\frac{\mu z^{2/3}}{E}\right) \quad \text{(for Au)}. \tag{4b}$$

Using expressions (1), (3) and (4) for both Al and Au, the transport elastic scattering cross sections defined as

$$\sigma_{\text{tr}} = 2\pi \int_0^{\pi} (1 - \cos\theta) \frac{d\sigma_{\text{el}}}{d\Omega} \sin\theta \, d\theta \tag{5}$$

has been calculated. Our results along with those of Ref. [3] are given in Table 1 and show a good agreement with each other.

Inelastic processes are handled in terms of Gryzinski's excitation function expression. For more details, we refer the reader to Ref. [12].

The simulation employs random numbers, all of which are taken from uniform distribution between 0 and 1. In Monte Carlo process, one chooses, on a random basis, the type of collision and the deflection angle and then moves the electron until the next collision a distance determined by the total scattering cross section, i.e., mean free path, for that process. The energy loss (in the case of inelastic scattering) is then obtained from the differential cross section as detailed in Ref. [12]. The angle of scattering was obtained from either the differential cross section or use of the binary collision model [13], depending on the type of collision, whereas the azimuthal scattering angle $\phi$ was uniformly chosen from the interval $(0, 2\pi)$. All the scattering calculations are carried out in a spherical polar coordinate system, where the $z$ axis is normal to the sample surface. The angle $\theta$ is taken from the $z$ axis, and the angle $\phi$ is taken from the $x$ axis to the projection of the velocity vector of the particle onto the $xy$ plane. This process is continued until the energy of the electrons is below a certain present threshold level (the electron is implanted) or until it has left the solid

Table 1
Transport elastic scattering cross section in units of Å$^2$ of electrons impinging on Al and Au

| $E_0$ (eV) | Al | | Au | |
|---|---|---|---|---|
| | Pw | Ref. [3] | Pw | Ref. [3] |
| 500 | 0.320 | 0.306 | 1.64 | 1.01 |
| 1000 | 0.110 | 0.115 | 0.810 | 0.709 |
| 1500 | 0.0568 | 0.0623 | 0.478 | 0.489 |
| 2000 | 0.0351 | 0.0397 | 0.318 | 0.359 |
| 2500 | 0.0240 | 0.0278 | 0.229 | 0.278 |
| 3000 | 0.0176 | 0.0206 | 0.174 | 0.223 |
| 3500 | 0.0135 | 0.0160 | 0.137 | 0.183 |
| 4000 | 0.0107 | 0.0128 | 0.112 | 0.155 |

Pw: present work, where the numerical coefficient depends on the electron incident energy.

(backscattered). In the present work, the termination energy is chosen to be 20 eV. The choice of the termination energy does not have much effect, since the path length travelled by the electron between 20 eV and near thermal energies is insignificant compared to the implantation depths [14].

It is clear that the backscattering coefficients depend sensitively on the details of the elastic scattering interaction since electrons typically have more than one lobe in the differential elastic scattering cross section [2]. This feature is, of course, strongest at low energies. The number of these lobes and their position depend on the material and the energy of the incident electrons [2]. Thus, a direct comparison of Monte Carlo simulation backscattering coefficients with experiments may serve as a test of the quality of the theoretical scattering models employed in this Letter. In order to evaluate the accuracy of the scattering cross sections employed in our program, we have calculated the backscattering coefficients for electron impinging on semi-infinite aluminum and gold with normal angle of incidence using total elastic scattering cross section obtained from a modified Rutherford differential cross section where $\beta_N$ is calculated according to relations (2) and (3), (4), separately.

Fig. 1. shows the variation of the electron backscattering coefficients as a function of its primary energy over the range 0–4 keV for Al and Au at normal incidence. Comparisons with experimental electron backscattering coefficients for both Al and Au have been made and reasonable agreement is found only when using relations (3) and (4). Moreover, our results generally coincide well with those of Dapor [3]. The good agreement between our Monte Carlo results and those obtained analytically by Dapor [3] indicates that, in the energy range of 500–4000 eV, the total elastic scattering cross section plays the main role in the determination of the backscattering coefficient. In addition, our results are closer to the experiment than those of Ref. [4]. The use of relation (2) shows clearly a disagreement with experiment and leads in the case of Au to backscattering coefficients that are too large as compared with experiment [9] which confirms the results of Ref. [1]. It should be noted also that our Monte Carlo backscattering coefficients and the experimental ones for Al have the same feature that backscattering decreases with increasing energy. However, for Au, the situation is completely different,

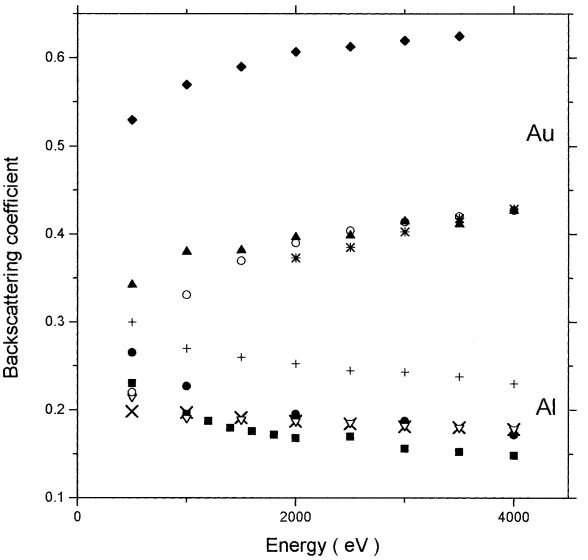


Fig. 1. Backscattering coefficient of electrons impinging on Al and Au as a function of incident energy. Filled squares: experimental data for the Al target (Ref. [15]). Filled circles: theoretical results for the Al target (Ref. [15]). Cross: theoretical data for the Al target (Ref. [3]). Plus: present work* for the Al target. Down empty triangles: present work** for the Al target. Empty circles: theoretical data for the Au target (Ref. [3]). Filled lozenge: present work* for the Au target. Up filled triangles: present work** for the Au target. Asterisk: experimental data for the Au target (Ref. [9]). *The numerical coefficients is taken to be constant. **The numerical coefficient depends on the electron incident energy.

since our Monte Carlo backscattering is larger than that of Al and increases with increasing energy following the same experimental backscattering behavior reported in Ref. [9] and the theoretical one obtained in Ref. [3]. This difference is explained by the fact that elastic scattering cross sections of gold atoms are larger than those of aluminium atoms and in elastic collisions gold atoms have a larger probability to scatter into large angles.

In summary, using a modified Rutherford differential cross section, where the numerical coefficient in the atomic screening parameter is taken to be dependent of the electron incident energy, for modelling elastic scattering in a Monte Carlo simulation, we have investigated the penetration of slow electrons in semi-infinite Al and Au. Our results for both Al (light element) and Au (heavy element) were in good agreement with the available experimental data and those reported in the literature using more complicated

methods for treating elastic collisions. This suggests that the screened Rutherford's cross section, which has been widely used in Monte Carlo simulations due to its simplicity and which was valid only for fast electrons, could be also used for slow electrons.

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