

BACKSCATTERING COEFFICIENTS FOR 8 – 32 KeV ELECTRONS: A MONTE CARLO INVESTIGATION

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Abstract. In this work, we present new Monte Carlo calculation results of the backscattering coefficients (η) for Al, Cu, Ti, Ag and Pt targets bombarded with monoenergetic normally incident electron beams having the impact energy E_0 between 8 and 32 keV. The simulations have been done with EGSnrc and Casino Monte Carlo codes. The EGSnrc values are in good agreement with those obtained with Monte Carlo code CASINO as well as with theoretical and experimental data taken from literature, showing that EGSnrc can be used for backscattering coefficients calculation, even if is a “Condensed history “ Monte Carlo code. This result encourages us to continue, in the future, with more complex applications of EGSnrc in the field of surface analysis.

Keywords: electron backscattering, Monte Carlo simulation, EGSnrc

1. Introduction

Studies of the laws governing the backscattering of primary electron fluxes are of particular interest for many experimental techniques involved in surface analysis like scanning electron microscopy, electron probe microanalysis and electron lithography [1].

Today, the main computational method used for calculating the backscattering coefficients is the Monte Carlo method. There are two types of Monte Carlo techniques involved in the transport of electrons/positrons through different media: (1) “Single scattering” Monte Carlo, also known as “analogue” Monte Carlo and used only for low energy transport, which follows each collision event sustained by each particle (2) “Condensed history “Monte Carlo which lumps many individual deflections of electrons against the nuclei of the medium into a single multiple scattering. In the field of surface analyses, in which are used electron beams having relatively low energies (5 to 35 keV), have been developed a number of simple “analogue” Monte Carlo codes, like NISTMonte, WinXRay, CASINO or MC-SET. The results obtained with these codes are good enough for the major part of the applications. Usually, the “Condensed history “ Monte Carlo codes, like PENELOPE, GEANT4, EGS4 (EGSnrc) or FLUKA are not involved in the field of surface analysis, even if these codes have

been partially benchmarked against experimentally measurements of electron backscattering at low energies.

Two different Monte Carlo codes have been used in this paper: EGSnrc and Casino. The EGSnrc (Electron–Gamma–Shower) system of computer codes is a general purpose package for the Monte Carlo simulation of the coupled transport of electrons and photons in an arbitrary geometry for particles with energies above a few keV up to several hundreds of GeV [2], while Casino [3] is a single scattering Monte Carlo SIMulation of electron trajectory in solid specially designed for low-beam interaction in a bulk and thin foil.

2. Materials and methods

When an electron beam impinges on a solid target, a fraction of the beam is absorbed, another fraction is backscattered, and the remaining one is transmitted. The sum of these fractions is equal to unity. Their values depend on the beam quality, the nature of the target and its thickness. The backscattering phenomena is usually described by the backscattering coefficient

$$\eta = n_{BSE} / n_B \quad (1)$$

where n_B is the number of incident beam electrons and n_{BSE} is the number of backscattered electrons. The backscattering coefficient strongly depends on the target atomic number Z and also slightly on the primary (impact) energy E_0 and on the incidence angle α [1].

A combined single-scattering [4] and diffusion [5] model of electron inelastic scattering has been developed by Niedrig [6]. Following Niedrig's approach, an accurate expression to calculate backscattering coefficient for normal incidence as a function of Z and E_0 was given by Dapor [7]:

$$\eta = 1 - (1 + 3\varepsilon\sqrt{Z-1}) / (1 + \varepsilon\sqrt{Z-1})^3 \quad (2)$$

where:

$$\varepsilon = 0.0811 + 0.0037E_0, \text{ for } 0 \leq E_0 \leq 6.7 \text{ keV, and}$$

$$\varepsilon = 0.1051 + 1.078 \times 10^{-4} E_0, \text{ for } 6.7 \leq E_0 \leq 45 \text{ keV}$$

In our simulations perpendicularly incident electron pencil beams with nominal energies between 8 and 32 keV have been forced to interact within five different metallic targets: Al ($Z = 13$), Ti ($Z = 22$), Cu ($Z = 29$), Ag ($Z = 47$) and Pt ($Z = 78$). The target thicknesses were fixed at 1 mm. For the EGSnrc simulations, the energy cut-offs for particle transport were set to $ECUT = AE = 512 \text{ keV}$ (kinetic energy (1 keV) plus rest mass), $PCUT = AP = 1 \text{ keV}$. Using EGSnrc for such low energy electron beams involves PRESTA-II for electron-step

algorithm, EXACT algorithm for boundary crossing, and “Spin effects” switched ON. The Casino code was used with default parameters. A number of 10^5 incident electrons has been used in all simulations (statistical uncertainties $< 0.4\%$).

3. Results and Discussion

The electron backscattering coefficients η at normal incidence as a function of impact energy E_0 for Al, Ti, Cu, Ag and Pt targets, calculated using EGSnrc and Casino Monte Carlo codes are given in **Table 1**.

The results have been compared with experimental data taken from literature [1]. Excepting the Al case, we found that both EGSnrc and Casino values somewhat overestimate the backscattering coefficient values reported by Yadav and Shanker [1] by several percents (up to 16% in the case of Ti target, when EGSnrc code was used, and up to 28 % for Pt target when Casino code was used). Generally, the best results have been obtained with EGSnrc Monte Carlo code, demonstrating the capacity of this code to calculate backscattering coefficients when transport parameters are fixed for low energy applications.

Table 1: Electron backscattering coefficients calculated in this paper. For every impact energy E_0 , in the upper line are given the EGSnrc values, the results obtained with the Casino Monte Carlo code being reported below. The percent deviations from the reference experiment of Yadav and Shanker [1] are given in parenthesis.

E_0 (keV)	Al (Z = 13)	Ti (Z = 22)	Cu (Z = 29)	Ag (Z = 47)	Pt (Z = 78)
8	0.167 (-2.9) 0.158 (-8.2)	0.259 (5.3) 0.267 (8.4)	0.319 0.331	0.394 (1.0) 0.445 (14.1)	0.473 (8.0) 0.560 (27.8)
12	0.165 (2.5) 0.146 (-9.6)	0.257 (6.6) 0.251 (4.3)	0.316 0.319	0.396 (2.1) 0.429 (10.6)	0.481 (6.7) 0.543 (20.5)
16	0.162 (6.6) 0.137 (-9.9)	0.254 (8.1) 0.244 (3.9)	0.311 0.307	0.404 (3.1) 0.422 (7.8)	0.489 (4.3) 0.535 (14.0)
20	0.159 (7.4) 0.134 (-9.3)	0.256 (11.8) 0.239 (4.4)	0.310 0.299	0.402 (2.0) 0.416 (5.6)	0.492 (4.0) 0.529 (11.7)
24	0.158 (12.1) 0.131 (-7.0)	0.254 (14.9) 0.236 (6.8)	0.312 0.297	0.402 (3.1) 0.411 (5.3)	0.497 (3.8) 0.528 (10.2)
28	0.155 (14.8) 0.130 (-3.8)	0.253 (16.1) 0.229 (5.1)	0.310 0.292	0.407 (3.8) 0.403 (2.9)	0.498 (3.1) 0.520 (7.6)
32	0.156 0.125	0.255 0.226	0.311 0.287	0.407 0.401	0.500 0.517

The Monte Carlo calculated backscattering coefficients have been also compared with older data reported by Hunger and Kuchler [8] as well as with the theoretical values

determined using equation (2) (see, for example, the **Fig. 1**). Good agreements have been found in all cases.

The general form of the $\eta = f(Z)$ can be understood by separating the electron–specimen interaction into an elastic component, which represents scattering through a significant angle without energy-loss and an inelastic component, which does not give the angular deflection, but it reduces the electron impact energy. The elastic scattering through a large angle increases as Z^2 , while the energy-loss has only a slight Z dependence [1]; thus, η is expected to be larger for heavier elements than for lighter ones.

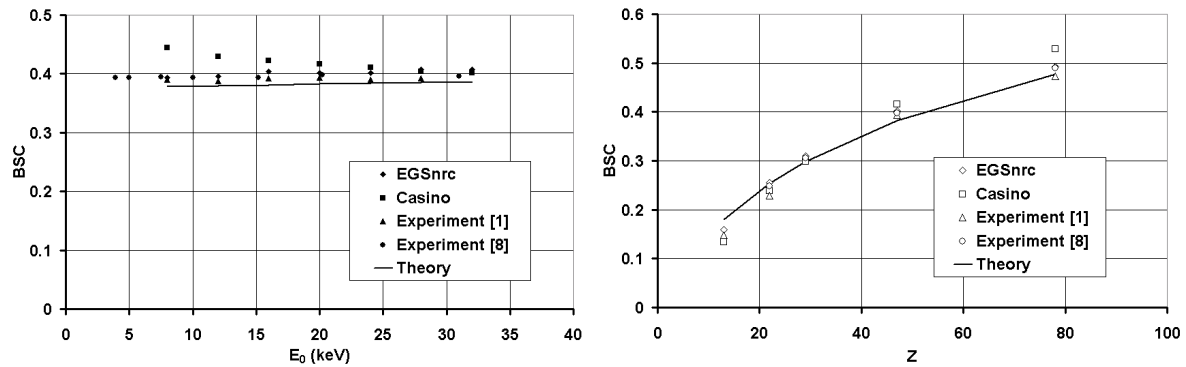


Fig. 1: Backscattering coefficients (BSC) η at normal incidence: (a) as a function of impact energy E_0 for a Ag target ($Z = 47$) and (b) as a function of atomic number Z at $E_0 = 20$ keV.

4. Conclusions

New Monte Carlo calculation results of the backscattering coefficients (η) for Al, Ti, Cu, Ag and Pt targets bombarded with monoenergetic normally incident electron beams having the impact energy E_0 between 8 and 32 keV have been presented. The EGSnrc and Casino Monte Carlo codes have been used and the results compared with other experimental and theoretical data taken from literature. Generally good agreements have been found, especially when EGSnrc code was used. These results encourage us to use EGSnrc Monte Carlo for more detailed investigations of electron-solid interactions.

References

1. R. K. Yadav, R. Shanker, J. Elect. Spectrosc. **151** (2006) 71.
2. I. Kawrakow and D.W.O. Rogers, **PIRS -701** (Ottawa: NRC) (2003).
3. P. Hovington, D. Drouin, R. Gauvin, Scanning **19** 1 (1997).

4. T. E. Everhart, J. Appl. Phys. **31** 1483 (1960).
5. G.D. Archard, J. Appl. Phys. **32** 1505 (1961).
6. H. Niedrig, Scanning Electron Microsc. **1** 29 (1981).
7. M. Dapor, Phys. Lett. A **151** 84 (1990).
8. H. J. Hunger, L. Kuchler, Phys. Status Solidi A **56k**, 45 (1979).