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A Monte Carlo Calculation of the Backscattering Coefficient for a Multilayer Sample

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Introduction

The Monte Carlo simulation technique has proven to be of great utility in the study of sample interactions in the scanning electron microscope (SEM). The method involves the calculation of the electron trajectory through a specimen in steps set equal to the mean free path between the scattering events. The appropriate scattering angles are chosen according to the type of event (elastic or inelastic) using random numbers and the trajectory is terminated when the energy decrease, due to inelastic scattering, approaches the original electron energy.

The signal derived from a multilayer sample in a SEM differs from a homogeneous sample in that the signal production and absorption are discontinuous. The differences depend strongly on the sample geometry, but can be calculated by the Monte Carlo technique if the layer thicknesses and positions can be taken into account. This situation can be approximated by averaging the calculated signal (Castaing 1960, Hermann and Reimer 1984) or by introducing correction terms to account for surface coatings (DeNee 1978, Hohn *et al.*, 1976, Niedrig 1982, Reuter 1972). To calculate the signal directly, however, the calculations must take account of the scattering differences at different locations within the sample. The calculation reported here was done using a Monte Carlo program originally created by Joy (1988) but the method can be applied more generally. The electron trajectories are monitored as they pass through the sample and the cross-sections for elastic and inelastic electron scattering are determined, at the specific energy that the electron has, at the location in the sample where the event occurs.

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Background

Incident electrons, which penetrate a specimen, change direction mostly because of elastic collisions with the atoms, but lose energy from inelastic collisions with the host electrons. Electrons which are backscattered escape the front surface of the specimen but these are also accompanied by electrons that have energies below the value at which it is sensible to terminate the calculation of a trajectory. To simplify the comparison of the calculations with experiment, the trajectory calculations were terminated at 50 eV and +50 volts was applied to specimens when the backscattering current was measured.

Elastic Scattering

Elastic scattering (Fig. 1) describes the collisions of an electron with the atomic nucleus. The mass difference between an electron and an atom is very large and so the direction of the electron velocity (v) can change substantially but the magnitude cannot. The elastic cross-section is described by a Rutherford model in the program written by Joy (e.g., Evans 1955) and is given by

$$\sigma_E = 5.2 \times 10^{-21} \frac{Z^2\, 4\pi}{E^2 \alpha (1+\alpha)} \left(\frac{E+511}{E+1024}\right)^2 \ (\text{cm}^2) \qquad (1)$$

where E is the electron energy, Z is the atomic number of the target atom, and α is a screening factor which has been estimated by Bishop (1976) as

$$\alpha = \frac{3.4 \times 10^{-3} Z^{0.67}}{E} \qquad (2)$$

The angle of scattering θ is determined from

$$\cos\theta = \left\{1 - \frac{2.\alpha.\text{RND}}{1+\alpha-\text{RND}}\right\} \qquad (3)$$

as described by Keyser (1982)

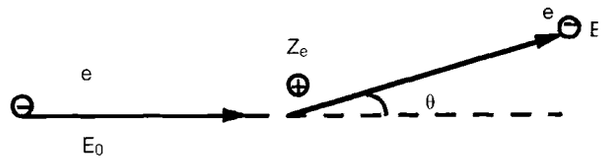


FIG. 1 Elastic scattering.

where RND is an equidistributed random number between 0 and 1. The mean free path between scattering events is calculated from

$$\lambda = \frac{A}{N_a.\rho.\sigma_E} \text{ (cm)} \quad (4)$$

where N_a is Avogadro's number, ρ is the density (g/cm^3), and A is the atomic weight (g/mol). This mean free path is the average distance that an electron will travel between elastic scattering events but the actual distance will vary. This variability is introduced by calculating the distance between the scattering events n and n+1 from

$$\lambda_n = -\lambda .\ln(\text{RND}) \quad \text{(cm)} \quad (5)$$

Inelastic Scattering

Inelastic scattering (Fig. 2) results from the collisions of the incident electron with the atomic electrons. In these events there is a significant amount of energy transferred to the target, with a concomitant slowing down of the electron, but the direction of the electron trajectory is not usually changed substantially. The continuous energy loss from these collisions is calculated using a modified version of the stopping power equation of Bethe (1930) due to Joy and Luo (1989)

$$\frac{dE}{dx} = -78500 \frac{\rho Z}{AE} \ln\left(\frac{1.16\,(E+kJ)}{J}\right) \text{ (keV/cm)} \quad (6)$$

where J is the mean ionization potential, given by Berger and Seltzer (1964) as

$$J = (9.76\,Z + 58.5\,Z^{-0.19}) \times 10^{-3} \text{ (keV)} \quad (7)$$

and k is a parameter which also depends upon the atomic number.

Backscattering Coefficient η

When a primary electron collides with an atomic nucleus the directional change can be quite large and a good proportion of the scattered electrons will be directed through the front surface of the sample. These electrons carry information about the sample composition because the angular distributions are dependent upon the atomic number [Eq. (3)]. The backscattering coefficient, η, is defined as the number of backscattered electrons (n_{BS}), divided by the number of incident electrons (n_B), i.e.,

$$\eta = \frac{n_{BS}}{n_B} = \frac{i_{BS}}{i_B} \quad (8)$$

Values of the backscattering coefficient, as a function of atomic number, have been determined by Bishop (1976) and Heinrich (1966).

The Multilayer Program

A Monte Carlo Program for Multilayer Samples

When a specimen does not maintain a uniform composition with depth there will be a variation in signal that is difficult to interpret. The case we have chosen to consider is that of a multilayer sample where each layer has a different composition, described in terms of the atomic number, atomic weight, density, and thickness. The program is designed to calculate the electron trajectories and the different interactions in each layer which depend upon the electron energy. The basis of the modification to the program derived by Joy (1988) for a personal computer is the determination of the energy and position of the electron in the specimen where each interaction takes place. The input parameters are necessarily more extensive and are introduced onto the computer screen by prompting the user to input the atomic number, atomic weight, thickness, incident energy, and the number of trajectories. An example of the screen format is given in Figure 3.

It is necessary also to modify the program so that the Graphics function initializes the screen and draws the beam trajectories. A schematic of the calculation and the

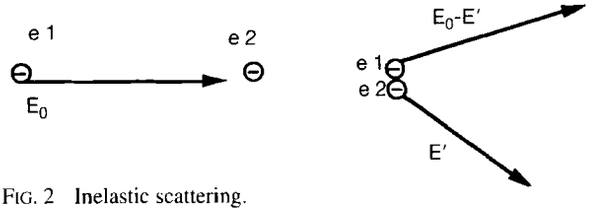


FIG. 2 Inelastic scattering.

Number of layers (15): 3 Beam energy (up to 100KeV): 20

Layer number	Atomic number	Atomic weight	Density (g/cc)	Layer thickness (Å)	Total thickness
1	28	58.71	8.90	1000	1000
2	13	26.89	2.70	1500	2500
3	28	58.71	8.90	1000	3500

Number of trajectories required: 100 Start to run: Yes

FIG. 3 Set-up screen to input data.

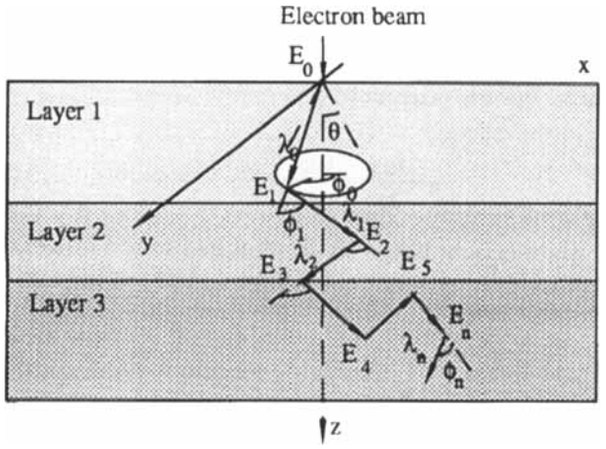


FIG. 4 Geometry of the initial step of electron scattering and energy loss.

geometry is shown in Figure 4 where E_0 and E_1 are the respective energies at positions 1 and 2, λ_0 and λ_1 are the mean free paths between the scattering events, θ is the scattering angle, and ϕ is the azimuthal angle.

The calculation of the trajectories is based on the parameters appropriate to the layer in which the electron interaction takes place and so the program has to be continually updated during the calculation of the electron trajectories. In order to account for an electron backscattering into a previous layer we have introduced a function which keeps track of and updates the position of the trajectory in the sample, rather than simply progressively changing the parameters. The proportion of backscattered electrons that escape from the surface is used to calculate the backscattering coefficient. The details of the entire calculation are shown in the flow chart (Fig. 5).

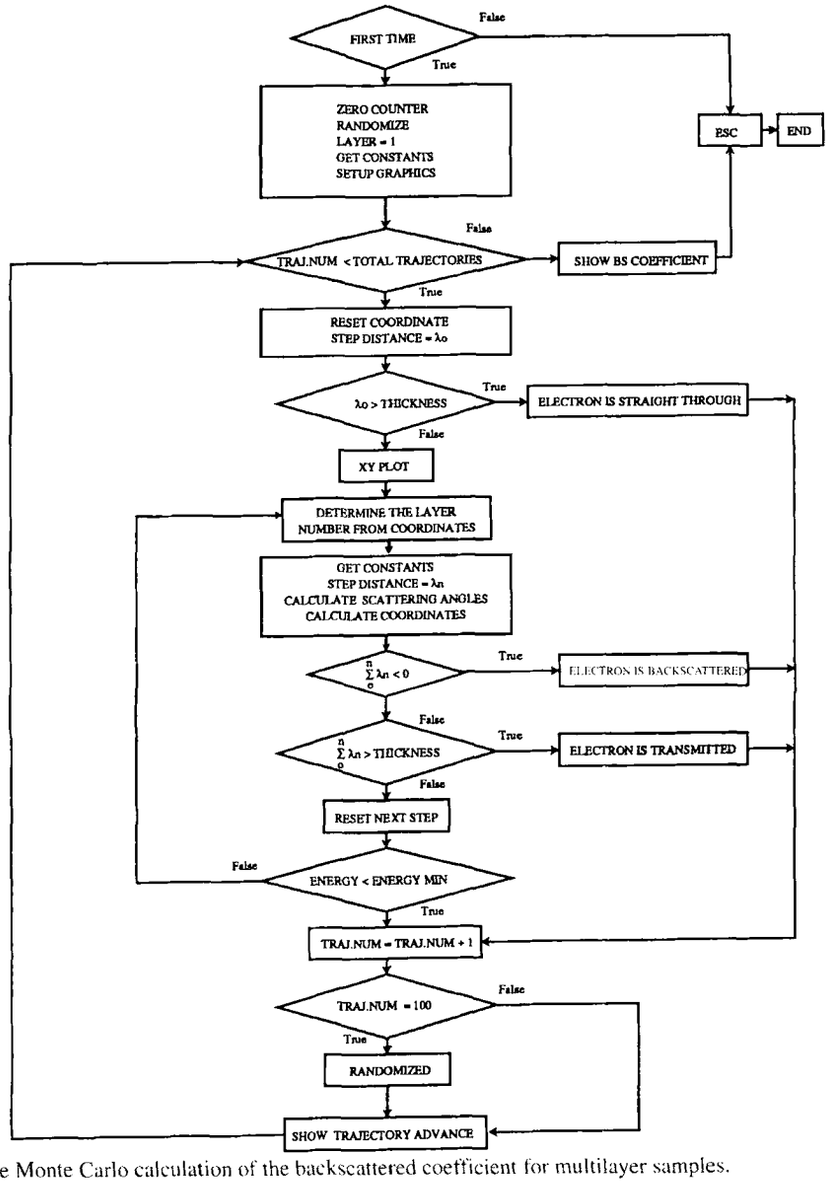


FIG. 5 Flow chart of the Monte Carlo calculation of the backscattered coefficient for multilayer samples.

Results

Calculations of the backscattering coefficient were made for a nickel aluminium multilayer sample 1250 nm thick (Ni 100 nm and Al 150 nm) at 10, 15, and 20 keV. A calculation is shown in Figure 6 at 15 keV and there is a difference in signal depending upon which layer is uppermost, hence two sets of data are shown in Figure 7.

A multilayer thin film of this thickness was prepared by electron beam evaporation and the backscattering coefficient was determined by biasing the sample at +50 V relative to ground. This reduced the escape of secondary electrons from the sample so that the backscattering coefficient η can be compared directly to the calculated value. The coefficient was determined experimentally according to

$$\eta = \frac{i_{BS}}{i_B} = \frac{(i_{BS} - i_{SC})}{i_B} \tag{9}$$

where i_B is the beam current, measured using a Faraday cup, i_{BS} is the backscattered electron current and i_{SC} is the specimen current.

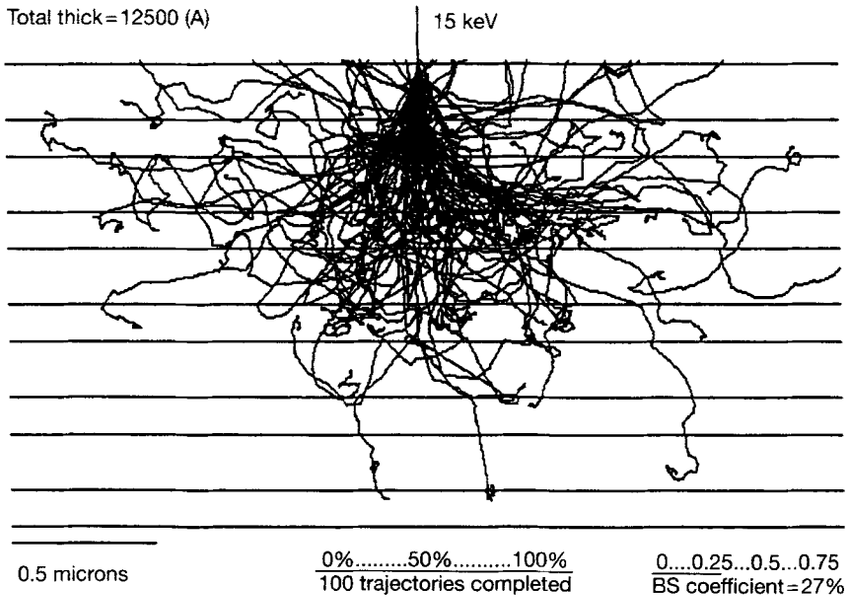
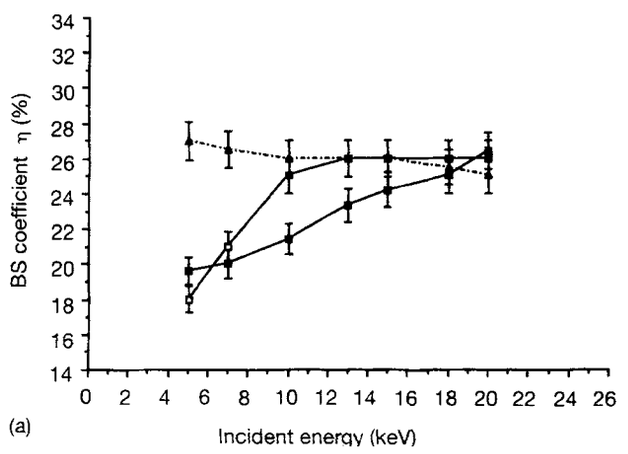
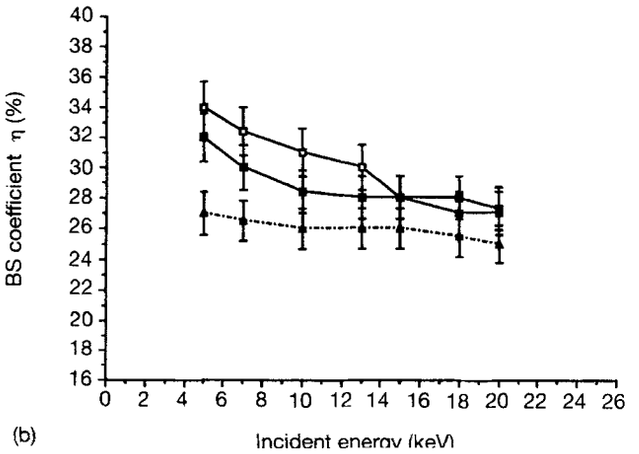


FIG. 6 The distribution of electron trajectories for a multilayer sample of Ni/Al with Al as the first layer. The Al layers are 150 nm thick and the Ni layers are 100 nm thick.





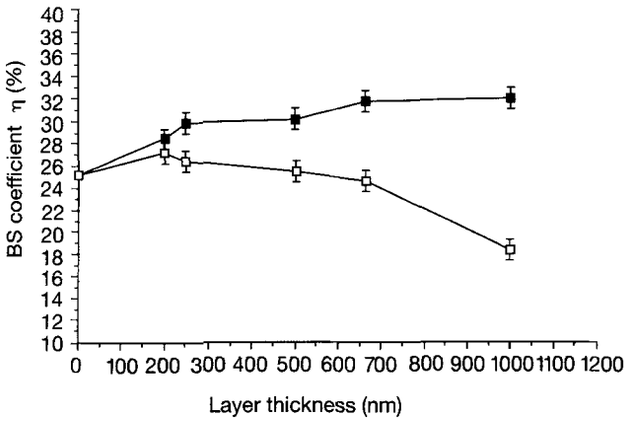


FIG. 8 Backscattering coefficient versus the layer thickness in a multilayer sample at 20 keV with aluminum ■ and nickel □ as the uppermost layers.

Summary and Conclusions

The backscattered signal from the aluminum nickel multilayer sample depends upon whether aluminum or nickel is at the front surface, but in both cases the signal is different from a homogeneous alloy of the same composition. In the calculations of the backscattered coefficient the homogeneous alloy is fairly consistent but both types of layered structure show a substantial variation (Fig. 7). The difference in the values of the coefficient are obviously less marked at high voltage, but they do persist and the values are quite consistent with the measured values.

Calculations of the coefficient as a function of the layer thickness, when both layers are the same thickness, are shown in Figure 8. It would seem that a fairly consistent determination of the layer thickness, in the 100 nm range, can be achieved by measuring the backscattering coefficient from such specimens.

Acknowledgments

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