

Monte Carlo Simulation of Electron Trajectories

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Introduction

This article presents a set of programs (called by the author **MC-SET**, that simulate electron beam trajectories in solid specimens, under conditions normally found in scanning electron microscopy (SEM).

As input the program takes the SEM operating conditions and a description of the specimen geometry and composition. It then computes and displays the randomly-scattered trajectories for a specified number of electrons representing the electron beam. For each electron it stores the dissipation of kinetic energy at each position along its trajectory. As its output, the program provides quantitative information about:

- electron trajectories in the specimen, e.g., penetration depth and lateral spread.
- electrons backscattered from the specimen, i.e. with high energy. It will also provide data on electrons transmitted through thin specimens.
- the 3-D distribution of the electron energy dissipated in the specimen, from which it is possible to calculate various of the signals measured with the scanning microscope, and hence, to emulate the contrast observed in images.

The flexibility in defining the specimens and the SEM parameters permits a wide variety of conditions to be simulated, giving, among other benefits, a better design tool for SEM work and analytical means for interpreting real-life experimental data.

Theory and Algorithms

Monte Carlo simulation is based on the complete evaluation of a large number of single interactions, each of which uses some random data as part of the calculation. The basic assumption in this method is that although the evaluation of parameters for a single particle cannot represent the actual process, a large number of such particles will be quantitatively and qualitatively representative.

The interactions between an electron and a solid can be separated into elastic and inelastic types. The former result in changes in the travel direction without changes in the electron energy, while the latter processes decrease the electron energy with a negligible change in direction.

In the **MC-SET** programs the electron travels a certain distance in the material during which it loses part of its kinetic energy, before being elastically (no energy change) scattered into a different direction. This process is repeated a number of times, until the electron energy has been reduced to a selected low, e.g. thermal, cut-off value.

Energy dissipation – inelastic scattering

The energy loss and the remaining energy of an

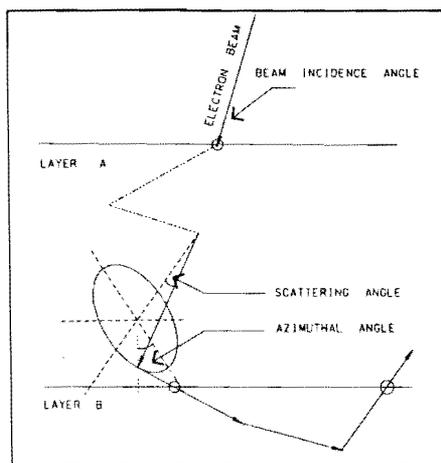


Fig. 1. Geometric definition of scattering angles; small circles: scattering parameters change as the electron moves to a different layer; energy deposition occurs at one extreme and middle of each trajectory step vector.

electron as a function of distance travelled in the material are evaluated using a modified form (1) of the original Bethe stopping power relation, dE/ds , valid for a wide range of electron beam energies.

This approach, as well as the original Bethe equation, takes account of all inelastic processes of the interaction, neglecting any change in the electron direction. It provides a differential equation in which the instantaneous electron energy change is related to the increment in trajectory step during the electron travel. Integration of the dE/ds relation over the path length provides two of the parameters needed for the simulation:

1. the Bethe range which is the maximum distance an electron will travel, until its energy is sufficiently small as to be indistinguishable from other thermal electrons in the specimen.
2. remaining energy of the electron as a function of trajectory path length.

Electron elastic scattering and trajectory step length

The change in direction undergone by the incident electrons (the scattering angle) depends mainly on the specimen material's elastic scattering cross section. The relativistic total-screened Rutherford elastic cross section is used (as in (2)).

Two scattering angles, shown in Figure 1, are defined: the scattering angle (ϕ) based on the Rutherford model, and an azimuthal scattering angle (γ), which specifies the trajectory direction on the cone with the solid angle of the scattering (ϕ).

In the **MC-SET** program, the angles in Figure 1 are calculated using the relations given in (2).

The scattering angle depends on the instantaneous beam energy, a screening factor, and a uniformly distributed random number. The azimuthal scattering angle (γ) is calculated assuming that the electron can scatter with equal probability (another random number) along a circle at the base of the cone defined by the ϕ scattering angle.

The distance travelled by each electron between scattering events is related to the mean free path between scattering events:

$$s = -\frac{A}{Nq\sigma_E} \log_e R_3 \quad (1)$$

where $\lambda = A/Nq\sigma_E$ is the mean free path in (cm), A is the atomic weight in (g/mole), N is Avogadro's number, q is the layer density in (g/cm^3), σ_E is the Rutherford cross section (in cm^2), and R_3 is another independent random number.

This method of following the electron path is called the *single scattering model*. The disadvantage of such an approach is the speed of calculation: the number of events (steps) considered for each incident electron is large, involving a relatively complicated calculation at each of them.

To increase the calculation speed the *plural scattering model* was developed. In this, the total length of the electron trajectory is assumed to be equal to the Bethe range (obtained through integration of the stopping power relation). This calculated range is then divided into a relatively small number of equal steps (for the present simulation this is taken as 50). The electrons are scattered only for this number of times, before completely losing their energy, or, until they are re-emitted from the specimen.

The azimuthal scattering angle (γ) is calculated as for the single scattering model, while the scattering angle ϕ in the plural scattering model is based on a relation due to Curgenven and Duncumb ((3), see for example (4)). This is also based on the Rutherford cross section, and as before, a uniform random number is used in the calculation.

Specimen description

The fixed coordinate system used in the simulation for the geometric definition of the specimen has the z -axis vertical, increasing downward, with the specimen top surface at $z=0$. The x and y directions are normal to the z axis (and therefore to the normal beam incidence direction). The y direction is specified to be in the plane of view (either the screen, or the paper hard copy).

Layers are assumed to be of rectangular shape and one on top of another, i.e., normally the bottom surface of the i -th layer is at the same z position as the top of the $(i+1)$ layer. This type of structure is commonly used in microelectronics

and optoelectronics devices fabricated by the planar technology method. For each layer, two pairs of y and z coordinates need to be specified.

At present, the maximum number of layers that can be used in a specimen is 10. Care must be taken to ensure that the specimen is continuous, with no empty areas. In this way, the program can be used for the investigation of the effects of precipitates, or the effect of beam excitation close to horizontal or vertical layer boundaries.

The plotting depth, called llz , is selected at the parameters input stage by trial and error, to represent the region in the device for which the incident electron energy dissipation is required. This approach involves running a number of quick preliminary simulations, with a small number of electrons and choosing the smallest value of llz for which the entire lengths of the electron trajectories are plotted.

Each layer in the specimen is defined by its atomic number, atomic weight and density. For specimens of mixed elements (compounds or alloys) the values for the atomic number and mass are the atomic mass weighted averages of those of the elements in the compound.

Energy dissipation and electron dose calculations

The energy deposited in the specimen for each step in the trajectory of each primary electron is equally distributed between two points along the trajectory step (as shown in Figure 1) to increase the 'resolution' of the energy deposition function. Energy deposition data is stored in an 80×80 matrix for a geometric volume of dimension llz . If at any stage of the calculation an electron moves to positions outside this region, its remaining energy is summed up in a value designated as *out-energy*, i.e. the energy not included in the energy deposition matrix or in the backscattered energy value. If it returns to the volume of interest, the program will carry on the calculations and deposit the electron's energy in the matrix.

Before the simulation begins one of the two possible types of energy dissipation matrix should be specified: either a radial cylindrical matrix with semi-circles concentric with the normal beam direction, or, a lateral matrix for planes parallel to the beam normal incidence direction. The selection of either depends on the specimen and experimental parameters, and on any further calculations to be carried out with the resulting data.

The total energy of the backscattered electrons (i.e., those leaving the specimen from its top surface) is calculated by summing the energy of all the emitted electrons.

The electron beam dose is defined as the energy deposited by the electron beam per unit length in the specimen. The *depth dose* gives the energy deposited per unit depth. It is the energy deposited in infinite slices parallel to the $x - y$ plane, per depth unit value. This is the most common dose type found in the literature, and is the one plotted on the right hand side of the graphical output of the simulation (see Figure 2). It should be stressed that the values given in this plot are for a *unit depth* of value $llz/80 \mu\text{m}$, where llz is the plotting depth input value given when defining the simulation parameters.

Examples of results

The simulation results presented here were obtained by running simulations with 3000

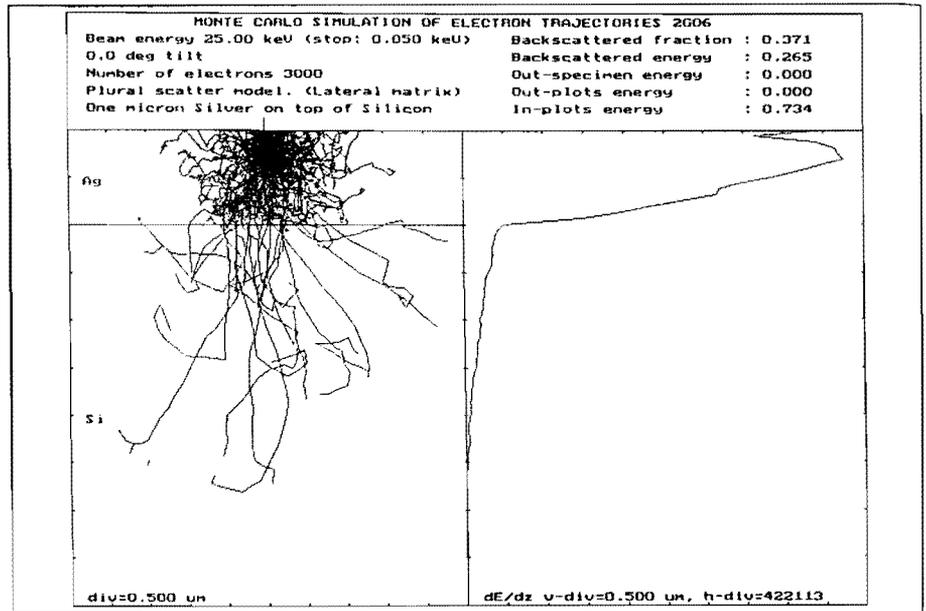


Fig. 2. Typical graphical output from the program.

electrons, using the plural scattering model. All the specimen materials parameters are already built-in the simulation programme, and only the specimen geometries had to be created.

Sample output of the programs

Figure 2 is an example of the graphical output obtained for a multi-layer specimen. The simulation was run on a 486 PC type computer, with a VGA screen and hardcopy obtained on a laser printer, taking less than one minute to calculate.

The left half of the figure is a plot of the first 200 electron trajectories used in the simulation. The horizontal line crossing the figure is the interface between the layers defined for this specimen, which is partially described in the comment above the actual plot. For single layer specimens and high beam voltages this plot resembles the well known 'pear shaped' energy dissipation cross section, but this is not the case, as seen, for multi-layered specimens.

The right side of Figure 2 is a plot of the depth dose function, i.e., the energy dissipated per unit depth. The shape of the depth dose, as a result of the two layers in the specimen, deviates significantly from the common analytical calculation (for example, the Everhart and Hoff depth dose function). It could only have been calculated by *Monte Carlo* methods.

At the top left of the plots, the parameters and comments used in the simulation are given. On the top right hand side some of the statistical results obtained in the simulation are given.

The backscattered coefficient, η , is the fraction of electrons backscattered from this specimen, i.e., 37.1% of 3000 electrons were backscattered.

The backscattered energy is the fraction of the beam energy leaving the specimen with the backscattered electrons, i.e., 26.5% of the total energy in the beam: $3000 \times 25 \text{ keV}$.

The *out-specimen-energy* is the amount of energy that escaped from the specimen, for example, with electrons leaving through the side faces, or transmitted electrons in thin specimens. In this example, the amount is zero.

The *out-plots energy* is the amount of energy deposited in the specimen, but not covered by the cross-section specified in the left hand side plot (as defined by the value of the plot depth specified). In this case, this amount is zero.

The *in-plots energy* is that calculated in the energy matrix: 73.4% of the total electron beam energy. With the other energies specified at the top of the right hand side plot, this should add up to unity.

Backscattering electrons

Figure 3 compares between backscattered electron data (iron at 20 kV beam voltage under different beam tilt angles) obtained using the *MC-SET* simulation and between experimental data from the literature (4). The backscattered coefficient (fraction) η is given both as lines drawn across the experimental values, and as points obtained by the *MC-SET* simulation.

The agreement between the simulated results with the experimental data presented in Figure 3 is very good for the whole range of tilt angles used. Further comparisons between simulated and experimental data of the variation of backscattering coefficient with atomic number agree within 10% of experimental values.

Materials properties and defects simulations

Defects or property variations in the specimen can give contrast in two ways in electron beam examinations: by changing the primary beam energy dissipation characteristics resulting, for example, in different dissipation volumes and backscattering data, and, by affecting the way that signals dependent on the energy dissipation are generated.

A foreign particle (precipitate) inside the specimen, for example, will affect the beam energy dissipation and the other signals related to it. Another example is presented in Figure 4 which gives the relative amount of the total electron beam energy dissipated in the semi-conducting layer (Silicon) of a dual layer specimen (Gold as the top layer, as in Figure 2) for various beam accelerating voltages. This parameter is important for the calculation of other signals, such

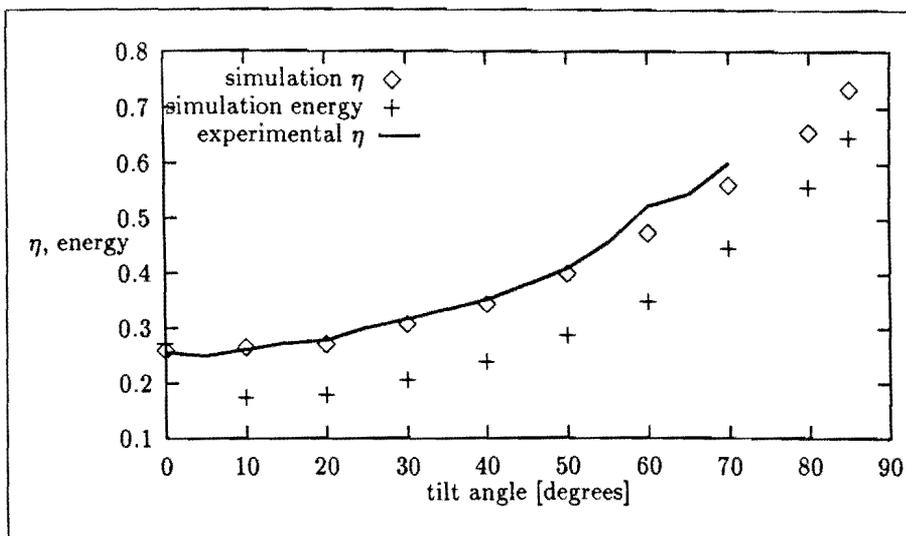


Fig. 3. Backscattered electron data for Iron as function of beam incidence (tilt) angle. Comparison between calculated and experimental backscattering coefficient η .

as, EBIC, X-ray and cathodoluminescence generation. In Figure 4, for each beam voltage (the horizontal axis), the energy backscattered and that deposited in the gold layer were subtracted from the total beam energy, to find the relative amount deposited in an underlying silicon layer (the vertical axis). Additional aspects related to the effect of thickness of overlayers on various signals can be found in (5).

An example of the second case above, where local changes in some physical property affects measured signals but not the beam energy deposition process, can be found in the study of dislocation contrast in EBIC (electron beam induced conductivity) microscopy (17). The energy dissipation volume calculated by *Monte Carlo* methods can be used to evaluate the charge collection current by modelling the dislocation as, for example, a region of reduced minority carrier diffusion length.

Additional applications of *Monte Carlo* simulations

In addition to their use in the study of the physical properties of the interaction of electron (or light) beams with matter, the simulations can be used for enhancing our understanding of signals related to these interactions. An example, partly dealt with in previous sections, is the evaluation of the backscattering coefficient η .

Among other types of signals found in electron microscopy, the following are currently being implemented using the MC-SET results for the three dimensional energy dissipation in the specimen.

Cathodoluminescence and X-ray generation

The calculation of the generation of cathodoluminescence (CL) depends on the specimen material(s) and the dissipation energy volume. In addition, corrections for absorptions and refraction from the layer surfaces should be included to give a reliable value of the intensity of light emitted.

X-ray intensity calculations present similar problems to CL. Their implementation allows for composition determination from multi-layers at various beam incidence angles and taking into consideration some form of ZAF corrections as used in electron probe micro analysis (EPMA). (*Monte Carlo* electron trajectory simulations on

mainframe computers were originally developed for X-ray calculations).

Secondary electrons

This procedure allows the calculation of the number of secondary electrons generated by the incident beam. Initial simulations for carbon specimens, for beam energies down to a few tens of eV provided very good fits to experimental data (6).

Biological applications

This *Monte Carlo* simulation article and the examples presented dealt with low primary beam energies, in the range of a few eV up to about 40 keV, as encountered in common scanning microscopy applications. Similar simulation methods are used for high energy electron beams, in the range of 0.1 MeV to 100 MeV, in medical radiation physics. For a general review of this subject see (8). It is found that the depth of penetration in water for monoenergetic beams is approximately 5mm per MeV of beam energy or about 3 orders of magnitude higher than the penetration depths found in scanning microscopy.

How to obtain the programs

The *Monte Carlo* programs are distributed by the

author to any interested individual. They are available only for PC and compatible machines, with a graphics display. In order to receive a copy, please send a cheque for £15.00 (or equivalent) to cover the costs of posting, disk (specify size required: 3.5 or 5.25 in), and a copy of the manual (which includes fuller descriptions of the physics and the calculation procedures used), to the following address:

Dr Eli Napchan, MC-SET Program Copy, Department of Materials, Imperial College, London SW7 2BP, England.

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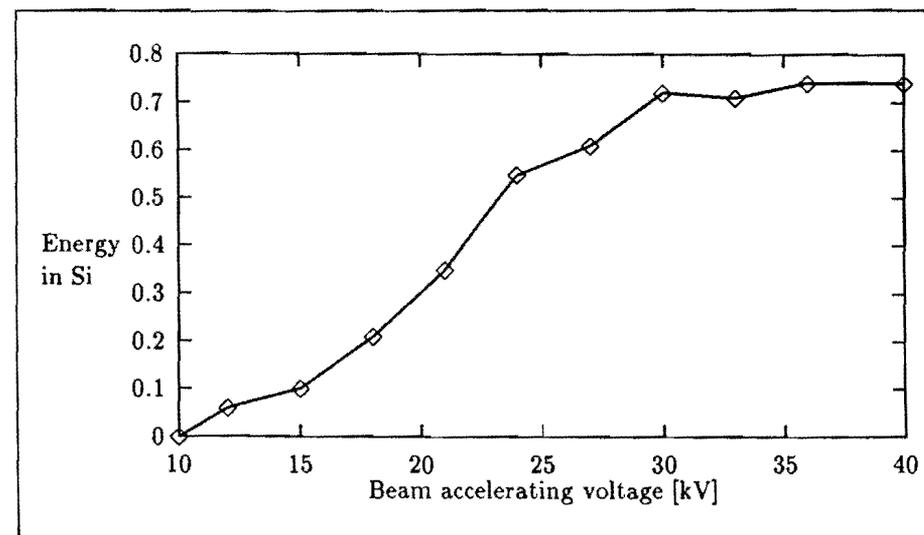


Fig. 4. Energy deposited in the Silicon layer with an overlayer of 2000 Å Gold, for various beam accelerating voltages.