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AN INTRODUCTION TO MONTE CARLO SIMULATIONS

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Abstract

The interaction of an electron beam with a solid can be modeled by the so-called Monte Carlo method. This technique produces a stepwise simulation of the electron trajectory by using random numbers to predict scattering angles on the basis of theoretical probability distributions or empirical models. The physical basis of electron scattering in a solid is described and two generic types of Monte Carlo model are then developed together with suggested examples of their application. An IBM PC compatible disc containing these programs is available from the author.

Key Words Monte Carlo simulation, electron scattering, stopping power, electron range, Xray generation, electron-hole pair generation, backscattering, secondary electron emission.

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Introduction

Increasingly electron microscopy is becoming a quantitative rather than a qualitative science. In order to correctly interpret images or spectra, however, it is necessary to be able to describe in detail the processes which produced that data in the first place and this is not a simple task because the interaction of an electron beam with a solid is highly complex. Before ultimately losing its energy or escaping from the specimen, each incident electron may undergo hundreds or thousands of separate scattering events, distributed between elastic and a variety of inelastic processes. While simple functional relationships can be derived between certain macroscopic properties of the interaction, such as the backscattering or transmission coefficients, and the parameters describing the specimen and the electron beam, the enormous number of different ways in which a given electron could complete the sequence of interactions involved in a single trajectory precludes the construction of a detailed analytic model. Monte Carlo sampling techniques, first used extensively by Von Neumann during the Manhattan project, provide a practical way of obtaining both macro- and microscopic descriptions of the beam interaction. The Monte Carlo technique uses random numbers as a means of predicting the magnitude of various events and as a way of selecting between possible scattering options. This paper describes how these methods can be implemented on personal computers with particular emphasis on their practical application to scanning electron microscopy.

Basic Principles of Monte Carlo Simulation

The Monte Carlo technique, as applied in this context, attempts to describe the trajectory which takes the electron through the solid. Although no individual trajectory produced by the simulation will represent a 'real' trajectory, if the physics of the processes encountered by the electron are properly modeled then predictions based on a large number of trajectories will accurately describe effects which can be experimentally observed. In order to make these calculations we need two basic pieces of information - the angles through which the electron is deflected as it travels in the specimen, and an estimate of how far (on average) the electron will travel given some particular value of incident energy. The simulations described here make two significant approximations in order to answer these questions:

(1) We assume that only elastic scattering events are significant in determining the path taken by any given electron as it moves through the solid. Elastic scattering, described by the screened Rutherford cross-section and produced by the

coulombic attraction between the negatively charged electron and a positively charged nucleus, results in angular deflections of from a few degrees up to 180°. The great majority of inelastic scattering events , on the other hand, produce angular deflections which are typically 1/2° or less. Consequently elastic scattering events are likely to be the ones which dominate in determining the path taken by the trajectory, and ignoring the effects of inelastic scattering introduces only negligible error while greatly reducing the number of computations that are required.

(2) The electron is assumed to lose energy continuously, at a rate determined by the Bethe (1930) relationship, rather than as the result of discrete inelastic events. This simplification allows the net result of all possible inelastic scattering processes to be accounted for without having to worry about the exact details of the individual events.

Neither of these assumptions is essential to the successful construction of a Monte Carlo program, and indeed much work has been put into simulations which specifically seek to avoid such radical simplifications. In practice, however, the benefits resulting from the gain in accuracy achieved by a more rigorous approach are usually outweighed by the substantial increase in computing time required. The procedures discussed here provide an acceptable degree of accuracy (i.e as accurate as a typical experiment performed on an electron microscope) while at the same time remaining capable of generating statistically valid data in a reasonable time period (i.e a few minutes to a couple of hours) on a personal computer.

The Single Scattering Monte Carlo Model

Within the constraints discussed above the most accurate Monte Carlo simulation of the electron beam interaction is one which attempts to account for each elastic scattering event suffered by the electron as it travels through the sample (Newbury and Myklebust 1981). We assume (figure 1) that the electron undergoes an elastic scattering event at some point represented by the coordinates (x,y,z), after having traveled from its previous scattering event. We wish to calculate the coordinates (xn,yn,zn) of the next point to which the electron is scattered. The parameters which describe the instantaneous situation of the electron are its energy E and the direction cosines cx,cy,cz of the trajectory segment that brought the electron from its previous scattering location to the point (x,y,z). These direction cosines are relative to a fixed set of axes attached to the specimen defined with the convention that the positive z-axis is normal to the specimen surface and directed into the specimen, the x-axis is parallel to the tilt axis, the x-y plane is the surface plane of a flat (i.e untilted) sample, and the y-axis completes a right handed set of axes. When the specimen is tilted the positive direction of the y-axis is down the surface of the specimen. To calculate the position of the new scattering point (xn,yn,zn) we need to know the distance between it and the point (x,y,z), and the elastic scattering angles ϕ and ψ.

The relativistically corrected screened Rutherford elastic cross-section σ_E is given by the relation

$$\sigma_E = 5.21 \times 10^{-21} \cdot \frac{Z^2}{E^2} \cdot \frac{4\pi}{\alpha(1+\alpha)} \cdot \left(\frac{E+511}{E+1024}\right)^2 \quad (cm^2) \quad (1)$$

where E is the electron energy (in keV), Z is the atomic number of the target, and α is a screening factor which accounts for the fact that the incident electron does not see all of the charge on the nucleus because of the orbiting electrons. Since it is difficult to predict a value for α theoretically we instead choose a value so that computed backscattering coefficients agree with those measured experimentally.Here the expression used is (Bishop 1976):

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

The elastic cross-section in turn defines a mean free path λ which is given by the formula

$$\lambda = \frac{A}{N_a \rho \sigma_E} \qquad (cm) \quad (3)$$

where N_a is Avagadro's number, ρ is the density (in gm/cm^3) and A is the atomic weight (in gms/mole). λ represents the average distance that an electron will travel between encountering elastic scattering events. Its value depends both on the beam energy and on the characteristics of the specimen, but is typically of the order of a few hundred angstroms at 100keV. Experimentally the actual distance that an electron travels between successive scatterings will, of course, vary in a random fashion. In our Monte Carlo simulation this variability is introduced by saying that the distance (or step length) between the scattering events at x,y,z and xn,yn,zn is given by the relation

$$\text{step} = -\lambda \log_e (RND) \qquad (cm) \qquad (4)$$

where RND is a equidistributed random number between 0 and 1 selected by the computer.

Figure (2) plots the variation of the step length, in units of λ , as a function of the random number chosen. Since the random numbers are uniformly distributed between 0 and 1 we see, for example, that there is a 10% chance of drawing a number such that RND<0.1 in which case the step will be equal to or greater than 2.3λ, and equally there is a 10% chance of picking a number such that RND>0.9 in which case the step length would be equal to or less than 0.1λ. The step lengths therefore vary over a wide range of values depending on the random number picked by the computer but, as can be verified by integrating equation (4), the average step length will be λ.

In the scattering event at (x,y,z) which marks the start of the step, the electron is deflected through some angle ϕ relative to its previous direction (see figure 1). The size of this deviation is determined by $d\sigma_E/d\Omega = \sigma'$, the angular differential form of the Rutherford cross-section and in the program is found by solving the equation :

$$RND = \int_0^{\phi} \frac{\sigma'}{\sigma_E} d\Omega \qquad (5)$$

where σ_E is the total Rutherford cross-section given above, and integration extends to a maximum value of ϕ. The right hand side of equation (5) represents the probability of the electron being scattered through an angle less than ϕ. Since we do not know, for any given scattering event, what the probability actually is we pull a random number RND from the computer, equate this to the probability and run the equation backwards to determine the angle for which this value would be correct. By evaluating equation (5), an equation can be derived (Newbury et al 1976) which relates the scattering angle ϕ to the random number RND:

$$\cos(\phi) = 1 - \frac{2\alpha . RND}{(1+\alpha-RND)} \qquad (6)$$

where α is the screening coefficient given above. This

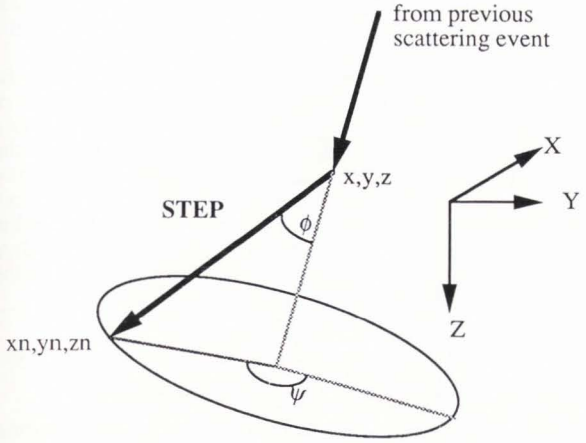

Figure 1. Coordinate system for Monte Carlo Simulation

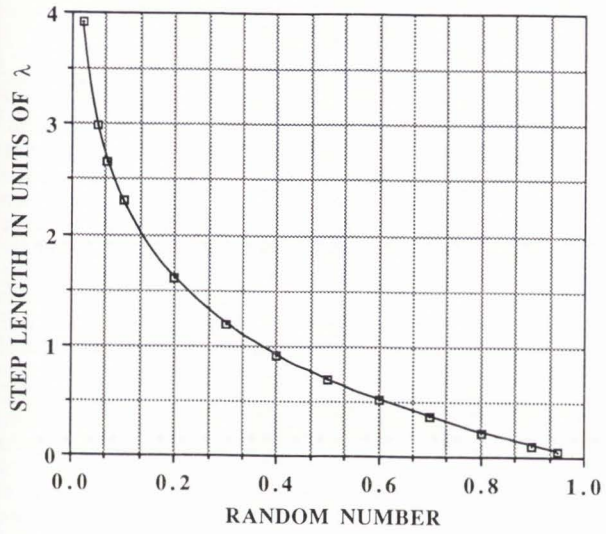

Figure 2 Distribution of step length with random number selected

equation generates a unique scattering angle in the range $0<\phi<180^o$, producing an angular distribution which matches that obtained experimentally. Although all angles between 0 and 180^o are possible, the great majority of scattering events are predicted by equation (6) to be less than 10^o. Figure (3) plots the probability of obtaining an angular scattering of greater than some minimum value ϕ for the case of a silicon target irradiated at 100keV. Note that while there is only a 1 in 10000 chance of an electron being scattered by an angle in excess of 110^o, more than 50% of all electrons are scattered through at least 1.5^o.

The electron can scatter to any point on the base of the cone shown in figure (1) so the azimuthal scattering angle ψ is given as

$$\psi = 2\pi.\,RND \qquad (7)$$

where, as before, RND is an independent random number selected by the computer.

All of the information needed to specify the scattering step from (x,y,z) to (xn,yn,zn) is now available. Although the calculation is straightforward, the algebra is cumbersome,

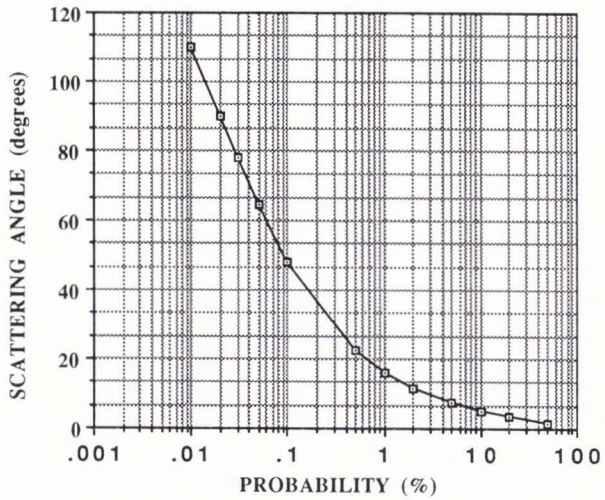

Figure 3 Angular distribution of scattering probability from equation (6)

because of the need to present the result relative to the initial fixed coordinate axes described above. Following Newbury et al (1976) we get:

$$xn = x + step.ca \qquad (8a)$$
$$yn = y + step.cb \qquad (8b)$$
$$zn = z + step.cc \qquad (8c)$$

where

$$ca = (cx.\cos\phi) + (V1.V3) + (cy.V2.V4) \qquad (9a)$$
$$cb = (cy.\cos\phi) + (V4.(cz.V1 - cx.V2)) \qquad (9b)$$
$$cc = (cz.\cos\phi) + (V2.V3) - (cy.V1.V4) \qquad (9c)$$

and

$$V1 = AN.\sin\phi,\ V2 = AN.AM.\sin\phi,\quad V3 = \cos\psi,\ V4 = \sin\psi \qquad (10a)$$

$$AN = -\frac{cx}{cz} \text{ and } AM = \frac{1}{\sqrt{1 + AN^2}} \qquad (10b)$$

Using this information the electron, given a starting energy, position and direction, can then be tracked through the sample a step at a time.

As it travels through the solid the electron loses energy and since the scattering is energy dependent we need to be able to compute the instantaneous energy at any time. The rate -(dE/dS) at which the electron transfers its energy to the material in which it is traveling is given by the Bethe (1930) relation:

$$\frac{dE}{dS} = -78500.\ \frac{\rho Z}{AE}\ .\ \log\left(\frac{1.166E}{J}\right) \quad (keV/cm) \qquad (11)$$

where J is the "mean ionization potential" which represents the average rate of energy transfer due to all possible inelastic events (i.e the production of X-rays, Auger electrons, secondary electrons, phonons etc). At sufficiently high energies (E>30 keV) J can be found analytically from the Berger and Selzer (1964) expression:

$$J = \left[9.76\,Z + \frac{58.5}{Z^{0.19}}\right].\ 10^{-3} \quad (keV) \qquad (12)$$

As E falls, however, the value of J also falls because some inelastic events which might contribute to its magnitude are now inaccessible. For example a K-shell ionization will not contribute to the value of J once $E<E_c$ where E_c is the critical energy and for a high Z material E_c may be tens of keV. To a very good approximation this problem can be taken into account (Joy and Luo 1989) by rewriting equation (11) in the form:

$$\frac{dE}{dS} = -78500 \frac{\rho Z}{AE} \log\left(\frac{1.166E}{J} + 1\right) \quad \text{(keV/cm)} \qquad (13)$$

This expression is accurate down to energies of 100eV or below and also avoids the difficulty that equation (11) cannot be evaluated for E<J. ΔE, the energy lost along the step from (x,y,z) to (xn,yn,zn) using either expression is then:

$$\Delta E = \text{step}.(dE/dS). \qquad (14)$$

The sequence of operations needed to simulate the electron path through the specimen can now be written out schematically in an algorithmic form:

repeat
Get starting energy E of electron
Get starting coordinates x,y,z for the step
Get direction cosines cx,cy,cz relative to initial axes
Compute mean free path λ for energy E and given material
Calculate the step length step from equation (4)
Find the scattering angles ϕ,ψ from equations (6,7)
Compute final coordinates xn,yn,zn from equations (8,9,10)
Compute finish energy E' = E - step.(dE/ds)
Reset coordinates x=xn,y=yn,z=zn
Reset direction cosines cx=ca,cy=cb,cz=cc
Reset energy E=E'
until electron leaves sample or falls below some minimum energy

This sequence of steps is then repeated to simulate as many electron trajectories as are required to produce data of the desired accuracy. The computer code to accomplish this sequence of operations is quite short, typically only requiring 50 lines or so in a language such as PASCAL, FORTRAN or BASIC. Addition of the code to provide such functions as a real time graphic display will, of course, make the program larger but overall program lengths even then rarely exceed a few hundred lines. On the disc, (for details see the end of this paper), the source code for this program in Turbo Pascal™ V5.0 is given in the file SS_MC.PAS, and an executable (i.e a compiled and runnable) version is in the file SS_MC.EXE

Applications

Figure (4) shows trajectories computed using the single scattering model for electrons traveling through 1000A° thick films of silicon and gold at 100 and 400keV . In this example the program, written in Turbo Pascal, was run on a Macintosh computer. Since at these energies the elastic mean free path λ is of the order of a few hundred angstroms, each electron will only be scattered a few times as it passes through the specimen, consequently only a few calculations per trajectory are required and the program runs very quickly. On an IBM AT-class machine equipped with an 8087 maths co-processor chip this program runs about 1000 trajectories or more per minute and significantly higher speeds are possible on 386 or MacII class machines. It must be noted again that we are not saying that any of the computed trajectories actually represents one that might be obtained experimentally under equivalent conditions. However, the representation obtained by averaging over a large number of computed trajectories produces data that is a good approximation to experimental reality. The relative error of a Monte Carlo simulation varies as $\sqrt{N}$, where N is the number of trajectories computed so an accuracy of a few percent requires the computation of several thousand trajectories. Consequently the time required to run 5000-10000 trajectories is an important measure of the usefulness of this approach.

By setting up appropriate criteria for detection, and the necessary code to count successful events, the fraction of electrons transmitted or backscattered by the sample as a function of the chemistry and thickness of the sample and the energy of the electron beam can be determined. In fact, since all of the possible information about every computed trajectory is available, we can also calculate information about other processes, such as the generation of X-rays or secondary electrons, initiated by the incident electrons. For example, the Bethe cross-section for inner-shell ionization is:

$$\sigma_x = 6.52\text{x}10^{-20}\left(\frac{1.8}{E\,E_c}\right)\log_e\left[\frac{0.65\,E}{E_c}\right] \qquad (15)$$

in units of ionizations/eV/atom/cm^2 where E_c is the critical ionization energy (in keV) of the X-ray line of interest. The X-ray production, I_s (photons/electron) along the step segment is then:

$$I_s = \sigma_x . \frac{N_a}{A} . \rho . \text{step}.\omega . f \qquad (16)$$

where ω is the fluorescent yield (photons/ionization) and f is the atomic fraction of the atom of interest in the compound. The X-ray yield from an element of interest can therefore now be found by including equations (15) and (16) in the computation loop given above, after first testing at each step that the electron energy E is greater than E_c. Even for the case of a single element target this computation is valuable because it permits both the lateral and the depth distribution of the X-ray production to be calculated. The program AEMMC, also included on the disk, uses the simulation described above and equations (15) and (16) to compute the spatial resolution of X-ray generation at the exit surface of a thin foil taking into account both beam spreading and finite probe diameter. The program plots the cumulative X-ray yield as a function of position relative to the beam impact point and by measuring the lateral distance over which this rises from 10% to 90% of its maximum value, a reliable measure of the X-ray spatial resolution is obtained. In the case of materials which are not homogeneous the Monte Carlo procedure is even more useful because the variation of X-ray production with incident beam position can be computed for a sample of arbitrary geometry and composition. For example, in the case of a material containing a boundary between two different phases, at each step of a trajectory the position of the electron is compared with the boundary position to determine f the atomic fraction of the element of interest. Equations (15) and (16) can then be evaluated as before, even making allowance, if necessary, for the differential mass-absorption caused as the X-rays from one phase leave the sample through the other phase. This computation can be performed simultaneously for each of the elements of interest.

Although the single scattering model has been illustrated by applications to thin foils it is not restricted to this special case and figure (5) shows an example of the use of the single scattering model to plot electron trajectories in copper at 20keV. However, the problem with this approach for bulk samples is that, even on a fast computer, the calculation is slow because a large number (typically 250 to 400) of interactions must be computed for each trajectory before the energy of the electron has fallen to a low enough energy, chosen in this case to be 0.5keV, for the residual range to be ignored. For many purposes involving bulk samples, therefore, a less rigorous, but substantially faster, model is applied and this is described in the next section of this paper.

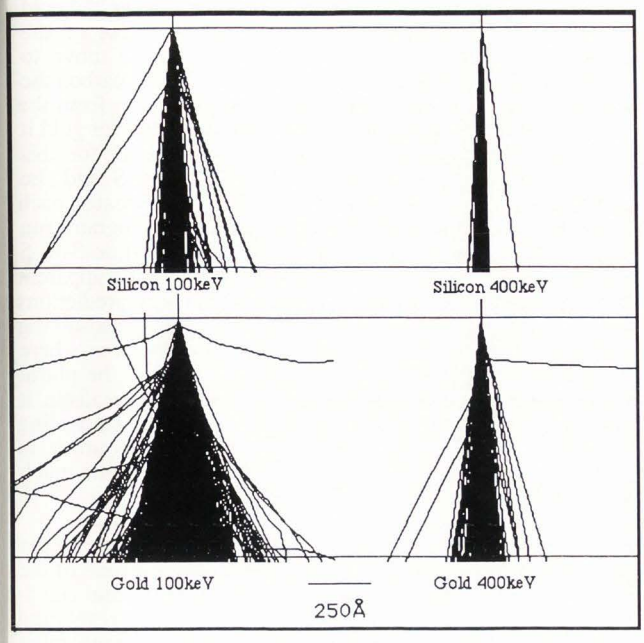

Figure 4. Monte Carlo simulation of electron trajectories in gold and silicon foils 1000Å thick, at 100 and 400keV incident energies. 250 trajectories are plotted in each example.

The Plural Scattering Model

The basic assumptions of the plural scattering Monte Carlo model are the same as those for the single scattering model, but the implementation is markedly different. The total length of the electron trajectory within the sample is taken to be the Bethe range R_B found by using Simpson's rule to numerically evaluate the integral:

$$R_B = \int_0^E \left(\frac{-1}{\frac{dE}{dS}} \right) dE \qquad (17)$$

where (dE/dS) is the stopping power given by equation (13). The Bethe range is then divided into, typically, fifty segments of equal length. This ensures that, unlike the single scattering case, there is a constant and relatively small number of computational steps associated with each trajectory. E[n], the energy of the electron at the start of the n^{th} step of the trajectory, is found by numerically solving the equation:

$$E[n] = E[n-1] - \int_{step} \left(\frac{dE}{dS} \right) dS \qquad (18)$$

where (dE/dS) is again obtained by the use of equation (11) and (13) in the appropriate energy ranges, E[1] is set equal to the incident beam energy E_0 and E[51] is set equal to zero.

The azimuthal scattering angle ψ is given by the same expression as previously used (equation 7) and the axial scattering angle ϕ is again described by the screened Rutherford cross-section but using a different formulation of the equation.. We write ϕ in the form:

$$\cot\left(\frac{\phi}{2}\right) = \frac{2p}{b} \qquad (19)$$

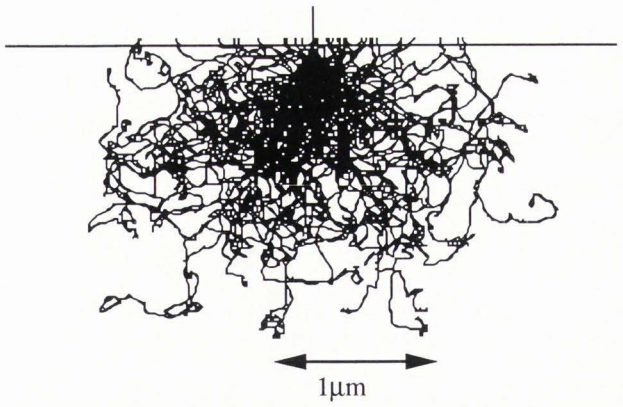

Figure 5. Electron trajectories in bulk copper at 20keV computed by the single scattering Monte Carlo model. 100 trajectories are shown.

where p is the impact parameter (i.e the projected distance of closest approach of the electron to the nucleus of atomic number Z), and b is $1.44 \times 10^{-2} Z/E$, where E is the instantaneous energy of the electron in keV. In each of the 50 steps making up one trajectory a large number of scattering events will occur (since the step length is now much larger than λ). Some of these deflections may add, and others may cancel so, following the original suggestion of Curgenven and Duncumb (1971), the net scattering angle ϕ is written as:

$$\cot\left(\frac{\phi}{2}\right) = \frac{2p}{b}\sqrt{RND} \qquad (20)$$

where RND is another random number between 0 and 1. In practice equation (20) has been found to introduce a systematic error into the simulation because it does not allow for a sufficient amount of small angle scattering. The equation is therefore rewritten as:

$$\tan\left(\frac{\phi}{2}\right) = \frac{b}{2p}\left(\frac{1}{\sqrt{RND}} - 1\right) \qquad (21)$$

in which form ϕ approaches zero as RND goes to unity. The final problem is in determining a suitable value for the impact parameter p. The approach used here derives from Love et al (1977) who rewrite equation (21) in the form:

$$\tan\left(\frac{\phi}{2}\right) = \tan\left(\frac{\phi_0}{2}\right)\left(\frac{E_o}{E}\right)\left[\frac{1}{\sqrt{RND}} - 1\right] \qquad (22)$$

where as before E_0 is the incident beam energy and

$$\tan\left(\frac{\phi_0}{2}\right) = \frac{0.0144\ Z}{2\ p\ E_0} \qquad (23)$$

ϕ_0 thus represents the minimum scattering angle for the incident electron with energy E_0. As can be seen from the functional form of the Bethe equation (see equations 11-13) the variation of (E/E_0) is substantially independent of the atomic number Z (the variation coming only from the mean ionization potential J which occurs inside the logarithmic term, and the random number RND will average to a mean value of

0.5 when a large number of trials is made). It therefore follows that the backscattering coefficient η should depend only upon cot ($\phi_0/2$). Experimentally this turns out to be a good approximation and we find that - for any element - the relation between tan ($\phi_0/2$) and the backscattering coefficient η can be written as a polynomial:

$$\tan\left(\frac{\phi_0}{2}\right)=0.016697+0.55108\eta-0.96777\eta^2+1.8846\eta^3 \quad (24)$$

To make equation (24) a usable one in the program we need an estimate for η for our target. This can be done by using a relation due to Hunger and Küchler (1979) which gives the backscattering coefficient η of a material of atomic Z at incident beam energy E as:

$$\eta(Z,E) = E^m C$$

where

$$m=0.1382 - \frac{0.9211}{\sqrt{Z}}$$

and

$$C=0.1904-0.2235(\ln Z)+0.1292(\ln Z)^2-0.01491(\ln Z)^3 \quad (25)$$

Given E and Z, then equations 24-25 give a value of η and hence of tan ($\phi_0/2$). (Note that if the target is not a single element but a homogeneous compound then the correct procedure is to find a value for η_{mix} - the backscattering coefficient of the compound- using the relation (Castaing 1960)

$$\eta_{mix} = \sum_i c_i \eta_i \quad (26)$$

where the c_i are the concentrations of the elements, $\sum c_i = 1$, and the η_i are found from equation 25, and then use this value in equation 24).

This Hunger-Küchler-Love-Cox-Scott procedure has the special advantage that the Monte Carlo simulation built around it can correctly predict the variation of the specimen backscattering coefficient with incident beam energy, an effect which is quite significant at energies below 5keV (Reimer and Stelter 1986). This is not normally possible with a model using a screened Rutherford rather than a Mott (Reimer and Stelter 1986, Czyzewski and Joy 1989) scattering cross-section. Although this procedure does not eliminate the need for the Mott cross-section, in many cases of interest (such as the production of X-rays or secondary electrons) the HKLCS approach does give an equally good fit to experimental data.The Monte Carlo loop then follows closely to the procedure described above and can be represented in algorithmic form as:

```
for n=1 to 50
    begin
     Get starting energy E[n] of electron
       Get starting coordinates x,y,z for the step
       Get direction cosines cx,cy,cz relative to initial axes
    Find the scattering angles φ,ψ from equations (21 and 7)
Compute final coordinates xn,yn,zn from equations (8,9,10)
       Check if the electron has been backscattered.
    If yes, exit the loop and add 1 to backscatter total
        otherwise:
          Reset coordinates x=xn,y=yn,z=zn
         Reset direction cosines cx=ca,cy=cb,cz=cc
end
```

Figure (6) shows trajectory plots computed for a 15keV beam into bulk samples of carbon, aluminum, copper and gold using this procedure. Note how both the size of the interaction volume and its shape changes as we move to progressively higher atomic number materials. For carbon the interaction volume is almost a cone hanging down from the surface, while for copper it is about spheroidal and for gold it is an oblate ('egg-shaped') spheroid. The source code for this program on the disc is in the file PS_MC.PAS and the corresponding executable file is PS_MC.EXE. Because each trajectory is now limited to 50 steps or less these programs run rapidly and on an IBM AT class machine the time 3 to 5 trajectories per second can be possible. Despite the apparent simplicity of this approach the agreement between predictions made using the plural scattering model and the single scattering model is generally excellent and except for a few cases where the granularity (i.e the size of the step length) of the plural scattering model is too high to permit a model to be realistic it is usually preferable to employ this technique when dealing with bulk samples since any slight drop in accuracy is outweighed by the gain in precision obtained from the much higher number of trajectories that can be run.

Applications

The plural scattering model can be applied in exactly the same way as the single scattering model, but the nature of the approximations made (particularly the limited - and fixed-number of the steps in a trajectory resulting in low resolution when the Bethe range is long) makes this approach most useful at low beam energies, i.e less than 20keV. It is therefore particularly adapted to SEM related studies. The type of model has been used to explain Type II magnetic contrast (Newbury et al 1976), to investigate low-loss images (Wells 1976), to quantify EBIC measurements (Joy 1986), to study secondary electron production in solids (Joy 1987) and even to characterize energy dispersive X-ray detectors (Joy 1985). An example of a typical application is given on the disc as the program PHIROZ.EXE. This displays the generation volume and relative density of generation of X-rays within a solid sample and computes and plots the $\phi(\rho z)$ curve (i.e the integrated variation of X-ray production with depth) for the material (Russ 1984). As interest in scanning electron microscopy continues to increase these sorts of tasks will become increasingly important.

Conclusions

Monte Carlo simulations of electron beam-solid interactions are powerful tools for the modern microscopist, and they are well suited for the age of the personal computer since the programs are compact and rapid in operation. A disc containing the Turbo Pascal™ (version 5.0) source code, as well as executable versions, of some of the programs discussed in this paper has been prepared. These programs will operate on any IBM PC or clone, with or without a maths co-processor, and with any of the common graphics cards. The disc contains a text file containing detailed instructions on running and using these programs. To obtain a free copy send a $5^{1/4}$" or $3^{1/2}$"disc, together with a stamped addressed disc mailer, to the author at the address on the front of this paper.

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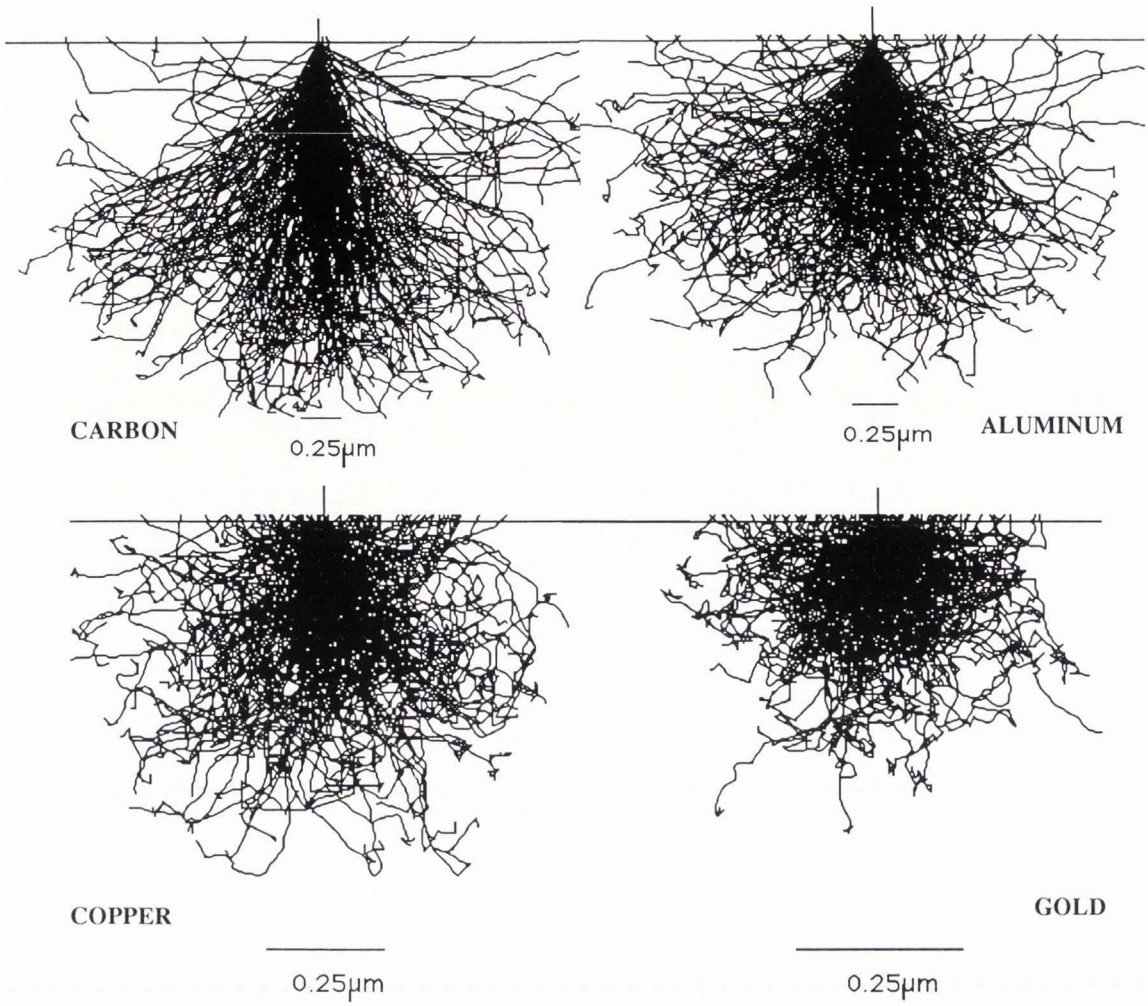

Figure 6. Monte Carlo simulations of trajectories in bulk samples of carbon, aluminum copper and gold at 15keV. 250 trajectories are shown for each example.

References

Berger M J, Seltzer S M (1964) Studies in Penetration of Charged Particles in Matter, *Natl.Acad Sci Natl Res Council Publ 1133*, 205-228

Bethe H (1930) Zur Theorie des Durchganges schneller Korpuskulerstrahlen durch Material, *Annalen de Phys.(Leipzig)*, **5** , 325-333

Bishop H E (1976) Monte Carlo Simulations, in *Use of Monte Carlo Calculations in Electron Probe Microanalysis and Scanning Electron Microscopy* , ed K F J Heinrich et al, (NBS Special Publication 460) , 5-15

Castaing R (1960) Electron Probe Microanalysis, in *Advances in Electronics and Electron Physics*, **13**, 317-386

Curgenven L, Duncumb P (1971) Simulation of Electron Trajectories in a solid target by a simple Monte Carlo technique, *Tube Investments Research Laboratories Report 303*

Czyzewski Z, Joy D C (1989) A Fast Monte Carlo for Electron Scattering in Solids, *J. Microsc.*, **156**, 285 - 292

Hunger H.-J, Küchler L (1979) Measurements of the Electron Backscattering Coefficient for Quantitative EPMA in the Energy Range 4 to 40keV, *phys.stat.sol., (a)*, **56**, K45-K48

Joy D C (1985) The EDS Detector - A quantitative model, *Rev Sci Instrum* **56** 1772-1779

Joy D C (1986) The interpretation of EBIC images using Monte Carlo simulations, *J. Microsc.* **143**, 233-242

Joy D C (1987) A model for secondary and backscattered electron production, *J. Microsc.* **147**, 51-64

Joy D C, Luo S (1989) An empirical stopping power expression for low energy electrons, *Scanning* **11**, 176-180

Love G,Cox MGC,Scott VD (1977) A simple Monte Carlo method for simulating electron-solid interactions and its application to electron probe microanalysis, J.Phys.D:Appl.Phys:, **10**, 7-23

Newbury D E, Myklebust R L (1981) A Monte Carlo model for analytical electron microscopy, in *Analytical Electron Microscopy 1981* , ed R H Geiss, (San Francisco Press:San Francisco), 91-98

Newbury D E, Yakowitz H, Myklebust R L (1976) The NBS Monte Carlo program, in *Use of Monte Carlo Calculations in Electron Probe Microanalysis and Scanning Electron Microscopy* ed K F J Heinrich et al (NBS Special Publication 460), 151-164

Reimer L, Stelter D (1986) Monte Carlo program for

minicomputers using Mott cross-sections *Scanning*, **8**, 265-274

Russ J C (1984) *Fundamentals of Energy Dispersive X-ray Analysis*, (Butterworths:London), 47-50.

Wells O C (1976) A Study of Low Loss Imaging, in *Use of Monte Carlo Calculations in Electron Probe Microanalysis and Scanning Electron Microscopy* , ed K F J Heinrich et al (NBS Special Publication 460), 139-150

Discussion with Reviewers

K.Murata Have you made a comparison between results obtained with the single scattering model and the plural scattering model over a wide range of energy? If so, could you comment on which model gives a better accuracy generally?

Author The relative accuracy of the two approaches depends on which parameters of the beam interaction are being simulated, and on the form of the specimen. In general when the specimen is solid (i.e non electron-transparent) then either approach can give equal accuracy for calculations of such global quantities as the yield of X-rays, or secondary, or backscattered electrons provided that appropriate precautions are taken. However, parameters of the interaction which depend on individual scattering events, for example the angular and energy distribution of backscattered electrons, will always require the use of a single scattering approximation. When the specimen is thin in comparison to the elastic mean free path length then only a single scattering approximation can be used.

K.Murata Could you comment on the accuracy of the models mentioned at very low energies, say 100eV?

Author The scattering models discussed here are not, in principle, suitable for incident beam energies below 1keV since at such low energies the Rutherford cross-section is not accurate and a Mott cross-section must be used (see for example Czyzewski Z and Joy DC, "Fast Monte Carlo method for simulating electron scattering in solids", J.Microsc. **156**, 285-291, 1989; Czyzewski Z et al, "Calculations of Mott Scattering Cross Sections", J.App.Phys., **68**, 3066, 1990). However, as noted above, for many purposes the difference in predictions between a simulation using the Mott cross-section and one employing a modified Rutherford cross-section is small because of the homogenizing effect of the plural scattering. The stopping power equation used here is only good down to about 50eV so computations in the low energy range will require a more detailed stopping power model.

K.Murata Is it possible for us to observe a group of electron trajectories e.g 100 trajectories on the display in a three dimensional way by rotating coordinates with your PC.

Author This is certainly possible to do since the start and finish x,y,z coordinates for each step of every trajectory are available. It would only be necessary to record these to a file and use a standard plotting program to display them.

G.Love How is the form of equation 4 determined ? One can see that the average step length will be λ if equation 4 is used but that does not necessarily mean the distribution of values about λ is appropriate.

Author The actual distance that an electron travels between successive elastic scatterings varies in a random fashion. The probability p(s) of an electron traveling a distance s when the mean free path is λ is

$$p(s) = \exp(-s/\lambda)$$

An estimate for the distance actually traveled can then be found by sampling this distribution with a random number RND, which involves solving the equation

$$RND = \frac{\int_0^s \exp(-s/\lambda)\, ds}{\int_0^\infty \exp(-s/\lambda)\, ds}$$

which gives

$$RND = (1 - \exp(-s/\lambda)$$

and hence

$$s = -\lambda \log_e(1 - RND) = -\lambda \log_e(RND)$$

(since RND is a random number between 0 and 1, 1-RND is also a random number in the same range and so can be replaced by yet another random number RND). This is the result of equation 4.

Y.Ho A Monte Carlo program implemented on a personal computer, and suitable for calculating secondary, backscattered, Auger electron, and X-ray yields for incident energies in the range from 3keV to 30keV, will be quite significant. What plans do you have to further develop the physical and calculation methods?

Author The programs discussed in the text represent the basic skeleton of a Monte Carlo simulation. The program disc available from the author contains examples of how this framework can be adapted to solve specific problems in electron microscopy. More generally further developments of the physical basis of these programs would involve the use of more accurate cross-section models (e.g a Mott cross-section), a more detailed stopping power model, and the removal of one or more of the major approximations identified at the start of the paper, for example including both elastic and inelastic scattering events in the trajectory computation. From a computational point of view the major advance is to take advantage of the very compact nature of the actual Monte Carlo calculation and to exploit this so as to achieve parallel computation on suitable machines. This would greatly reduce the time required to achieve adequate statistical accuracy and enhance the utility of these methods.

P.Rez Your statement in the introduction is too strong. It is certainly possible to write down a transport equation describing all scattering in a solid. The equation might not have a closed form analytic solution when the boundary conditions are applied.

Author You are correct. The reason why Monte Carlo methods rather than transport theory calculations have become common tools is not that the Monte Carlo method is more accurate or rigorous, but that for typical practical situations a transport theory solution is too complex to be tractable.

P.Rez I object to the use of the word "predicting" to describe the application of distributions generated from Random Numbers. To be strictly accurate the Monte Carlo distribution simulates the electron scattering provided that the statistical sampling has been done correctly.

Author Correctly this method is called Monte Carlo sampling because random numbers are being used to select between various options on the basis of their relative probability. The simulation follows from this sampling. In the earliest Monte Carlo work on electron interactions the scattering distribution was not, in fact, generated by the computer at all, instead a measured experimental distribution was sampled by the random number generator.

P.Rez I have always been unhappy at the circular arguments used by the Monte Carlo community. The screening parameter is fixed to give the correct backscattering coefficient, so one should not be surprised if the subsequent calculation gives the correct result for quantities related to backscattering. I should

also point out that the prescription of Curgenven and Duncumb is not based on any proper treatment of multiple scattering. The justification appears to be that as the calculations gives results in agreement with experiment then it must be right.

Author The 'circularity' of the argument is unavoidable because many of the parameters needed to perform the computations are not available even to a first approximation. Fitting the computed yields to experimental backscattering values provides a way of replacing the unattainable microscopic data by a piece of readily available macroscopic data. The proof that this procedure is viable is not that it then reproduces the backscattering yield that it was originally normalized with, but that it correctly predicts the behavior of this and other parameters of the electron beam interaction under conditions that are quite different to those used to produce the initial agreement.The Curgenven and Duncumb treatment of multiple scattering was not intended to be rigorous, rather it was a device to permit rapid evaluation on the rather small computer then available. However their approximation is neither unreasonable nor unphysical, as evidenced by the fact that removing it and replacing it by a proper treatment actually produces little substantial increase in accuracy for the majority of conditions. Since we are sampling a distribution it is not necessary to know, or be able to reproduce in detail, the exact mechanism by which this distribution is obtained. We are only required to be able to state with sufficient accuracy what form the distribution takes.