Fall 2003 Monte Carlo Assignment

Purpose
The goal of this exercise is to get you to “think like an electron”.... to start to think about where electrons from the stream of high energy electrons go when they hit the metal or mineral or semi-conductor or glass you are analyzing. Where do the electrons go in the process of generating x-rays? How big of a region do the x-rays come from? What factors govern the size of this “interaction region”? (Think ... spatial resolution). Do all x-rays in your sample come from the same region? Do the backscattered elections come from the same region? What about secondary electrons?

Introduction
At some point (it doesn’t matter whether before, during or after), please read the 1991 paper by Joy (An Introduction to MC Simulations) to get a better understanding of what these programs are modeling.

We will be using 2 of the programs on the Goldstein book’s CD: they are in Ch 3; and also copies are now on the G777 web page. The first one is in the CD’s MC_Windows folder – copy all 3 files to a folder on your hard disk. The second one is in in MC subfolder within MC_CTF, then copy the MC_95.zip file to another folder on your hard drive and unzip it. (These programs run under Windows. The older versions that we previously used would run under DOS or Mac (OS 9). In a pinch, you still could run them.)

Open or print out the “ReadMe.doc” for the first program. This is a 7 page introduction and exercises for Joy’s MC_Demo - MC Modeling for WIN98.

The first program (McforVB, Monte Carlo for Visual Basic) is great for demonstrating most of the points here, but is limited in not allowing any direct input of compositions, rather you have a limited set of mainly pure elements to select from. The second program (SS_MT_95.exe) allows you to input anything, which we want to do for the second part of this exercise, to look at two “real minerals”, quartz and magnetite.

Exercises:
I have limited the number of cases for you to test out--use the values I give below rather than those Joy give. Answer all questions in Joy’s text for the relevant sections, plus ones I give below. n.b. All models are scaled to fill the screen, but the scale bar can be vastly different. Observe it to make spatial estimates.

Also, let us use a convention that defines the electron range (the measure of the extent of the interaction volume) as the distance from initial impact to an eyeballed 90% of the maximum distance (and since so much is in the dense center, this really is something like 95-98%)

4 Exercises with McforVB:

(1) WALK
Do all exercises listed

(2) AEM (Analytical Electron Microscopy, i.e. TEM
As we are mainly interested in SEM and EPMA, not TEM, we will only do section (c), modifying the thickness to 5000 angstroms (making it similar to the thickness of a small inclusion in your sample). See what happens as you reduce the voltage from 100 keV down to 5. Try to determine precisely what voltage is the highest you can use to make the foil act like a bulk specimen (to the nearest tenth keV).

(3) PS
(a) instead of C, Cu, Ag and Au, do C, Si, Cu and Au. Make a table of the electron ranges. Also compare/contrast the overall shape change from low Z (C) to high Z (Au)
(b) only do for Cu
(4) SS
Do as listed (repeat the same calculations done in (3) above; is there any/much? Difference in the results using this more exact procedure?.

1 Exercise with SS_MT_95.exe

(5) SS
Using 250 trajectories, at 15 keV, run simulations on SiO2 (quartz), Fe3O4 (magnetite). Determine and compare the electron range (Interaction volume) and the BSE coefficient for them. (assume quartz density=2.65, magnetite 5.20 g/cc). Calculate mean atomic number and weight per method given below.

How to calculate Mean Atomic Number for a compound: there are several (different) variations on how to do this. Some suggest scaling the elements in the compound by the atomic proportion of the element, but the method I believe is the most correct is the one utilized by David Joy, which is to scale by the weight proportion of the element.

Example: Quartz, SiO2
First, determine the wt proportions (fractions):
Si = 28.09
O = 2 x 16 = 32.00
Total wt = 60.09
Thus Si = 28.09/60.09 = 0.4675
O = 32/60.09 = 0.5325

So, for the mean atomic number we scale
Si At number (14) scaled by its weight fraction 0.4675 = 6.55
And add to that
O At number (8) scaled by its weight fraction 0.5325 = 4.26
Summing these up gives 10.81 as the mean atomic number of SiO2 (also some use the abbreviation Z bar)

How to calculate Mean Atomic Weight for a compound: You sum up the total atomic weight (multiply each element at wt by number of atoms, summing up over all elements), then divide by the total number of atoms in the compound. So for SiO2, you divide 60.09 by 3 and get 20.0

Summary Paragraph
Summarize the effect of accelerating voltage, and of composition (Z) on the amount of electron scattering/interaction volume.
How do the physics of the process affect your attempt to analyze a small (micron-size) grain? If you had a 5000 angstrom (0.5 micron) thin film of copper on a substrate of Al, what would be the maximum accelerating voltage you might want to use to be sure you stay in the top film?