Geology 777 – Monte Carlo Exercise II

This week we will continue to utilize Monte Carlo simulations. Specifically, we will use the CASINO (Windows) application. It can be downloaded from either the class web site or its homesite **www.gel.usherb.ca/casino/**. The name is from "monte CArlo SImulation of electroN trajectory in sOlids" , and was originated by Raynald Gauvin of Univ of Sherbrooke (Quebec). Be sure to run it from a folder/directory which contains the "int" folder at the same level as the .exe file.

There is an article in 2007 Scanning on this program which you should look at (posted on the class website).

The program models both the electron scattering and the X-ray production by those electrons, and is quite useful for determining what kind of accelerating voltage must be used to keep the electrons and the x-rays within the top layer. However, it does NOT consider the problem of "fluorescence across phase boundaries", which we will consider in the future.

It is set up to simulate both bulk specimens, plus 2 different physical specimen types: thin films (could be more than one) over a substrate, or a specimen with vertical phase boundaries, e.g. lamellar structures.

You have 3 problems:

1. Compare the electron scattering and x-ray generation in Si and SiO2 solids.
2. Look at the problem of having a thin (1 micron) lamella of SiO2 surrounded by Fe3O4
3. Look at several thin films

I. Bulk Sample of Si metal

Instructions for Bulk Samples:

1. Run Casino v. 2.42

2. File-> New, automatically opens Edit Layers dialog box, click Add Layer, then select the Undefined (=Substrate) and type in Si (case sensitive) and it should put in the proper density for the metal. Click Done. Then click Next.

3. You are now in the Microscope and Simulation Properties dialog box. There are only 3 things to edit here:

   a. Define the accelerating voltage (we only use a contant one): Start, change from 1 to 15 kV,

   b. Number of electrons to simulate, default is 200 which is good for the first couple of runs you do to make sure you're doing it correctly, but really gives poor statistics. Once you have figured out how the program runs, you want to set up longer runs (5000) and on most modern computers will take <45 seconds.

   c. Beam radius (nm): default 10 nm is for an SEM; for BSE with typical electron probe, can use a larger beam (say 100 nm), but leave the 10 nm as this will not really matter much as far as the final results in BSE, CL or x-ray images.

   d. Click Next --> to go to next setup box.

4. Distributions Dialog box. Generally leave this alone. Click Next --> to got to next setup box.

5. Options Dialog box. Here you may wish to increase the number of displayed trajectories (on screen), default is 200, but set to 5000. Leave rest alone. Click Next -->

6. Select Physics Model; here you can "peak under the hood" to see that there are many models for the various physical processes being modeled. Leave it alone. Click Finish.

7. You now get a New Simulation Request box. Click Yes. And away it goes.

9. Active display. At the bottom of the active window will be a timer showing elapsed time, and also a running calculation of the backscattered electron coefficient. There will be an actively updated display of incident electrons (blue) and backscattered electrons (red) up to the max number you specified in Options Dialog box above. The display is actually a relatively constant sized interaction area, but what is different about different specimens is the lateral and depth scales (beware, numbers are in nanometers). For our example of a lamella, it is nice to be able to reduce the scale to see the position; you can do this under View --> adjust scale, setting the x axis to 4000 or more nm (also the second button from right on toolbar). Wait for the simulation to finish.

Questions: what is the BSE coefficient (as fraction)? _____ Having scaled the display, eyeball the maximum dimensions (=ranges) of the inelastically scattered electrons (blue ones), not using any single outlier, but a value ~90% of the furtherest electron. Electron range in Z _____ nm
Radial electron range in X _____ nm

10. On the left column is displayed a folder labeled with the accelerating voltage. Click +, and then underneath (inside) are subfolders labeled Distribution, X-Ray, and X-Ray Radial Distribution. You want to save this run now to some folder you create on your computer, as you may want to come back and re-examine the run later.
Open each option up one by one.

11. Distribution -- of electrons (potentially all: backscattered, transmitted, secondary)

1. ZMax--maximum Z penetration of ALL electrons (low relevance here)
2. ZMax Backscattered--max Z penetration of Backscattered Electrons (low relevance)
3. Backscattered Energy--histogram of spread of BSE energies (low relevance)
4. Transmitted Energy - irrelevant in this geometry
5. Surface Radius of BE--key data, this is the BSE spatial resolution. Question is how to interprete the "edge" of the BSE signal. I suggest the cumulative 90% of the signal (as it tails off on the outer limits for a bit.
6. Energy of Surface Radius of BE--low relevance here
7. Energy by Position--very important for consideration of the maximum extent of the lowest energy electrons that can cause CL to occur in the specimen. The concentric shells show the remaining energy level, and there are faint grayish boxes that show the maximum extent.

Questions: For electrons with a maximum (remaining) energy of 3.75 keV, what is their maximum depth? ____ nm maximum lateral radial spread from the center line? ___ nm. Now consider the energy needed to produce Si Ka xrays… which is _____ kV. The red line is close to that level, what is the maximum depth at which there are electrons with this energy? ____ nm
Maximum lateral radial spread from the center line? ____

12. X-Ray -- these are the Phi Rho-Z distributions (intensity of x-rays vs depth in nm), with Blue showing the x-rays generated that do not escape the sample **(normally called Generated**, but here called "Non-absorbed"), and Red showing the x-rays that escape from the sample and reach the detector (**normally called Detected or Emitted**, but here called "Absorbed" apparently using non-uniform terminology, referring to x-rays absorbed by the detector—very confusing!! Sorry.). Notice that the lower energy x-rays suffer greater absorption (IN THE SPECIMEN!) and only those near the surface escape. The next set of X-ray plots which show the surface radial distribution of x-rays. (Phi = x-ray generation function; Rho-Z is one way to plot generation, per unit density at discrete depth

slices). Note that here and in virtually all samples, the maximum intensity (y axis) is at some fraction of the total depth (x-axis).
--Click on an element (listed alphabetically) and in some cases the excitation energy (e.g. 15 kV) can excite 2 separate families of x-ray lines (K, L, M etc).

Questions: Click Si-K: At what approx. depth is the maximum depth (99%) of Si K x-ray production? ___ nm. Note that 2 numbers are given for Blue (Generated) and Red (Emitted). Calculate the percentage of Emitted relative to Generated (red divided by blue as percent). _____

13. X-Ray Radial Distribution-- here is the lateral (radial) expression of the x-rays generated at depth. Most of the x-rays are generated within some small radius of a projection directly below the point of impact on the surface, but there will be lateral scattering, and always be a "tail" extending far out.

14. The program unfortunately does not display the x-ray radial data on a log scale, and thus it is hard to see the maximum radius within which the majority (e.g. 99%) of the x-rays are generated. To do this, you have to first display a particular display (e.g. Si k) and then manually export it to a file -- Distribution→ Export Data; save as a named file, and open in Excel, then normalize (using the maximum counts, here the first row value) the generated (2^{nd} column) –make a 4^{th} column * 100 to get percents, then normalize the emitted (3^{rd} column)-make a 5^{th} column *100 to get percents.
Just look at the data and you can see where you are at the 1% intensity level (=99% of xrays are within that radius). If you want, plot as scatter, then display Y as Log scale.

Questions: 99% of all Si Ka xrays come from a maximum depth of ____ nm.
And 99.9% come from a maximum depth of ___ nm.

II. Change the Si to SiO2: Now, run SiO2 in the same way (density = 2.62). Is the electron range (a) much greater, (b) much less, (c) about the same? ____

Look at the X-ray phi-rho Z plot for Si Ka. : At what approx maximum depth (99%) of Si K x-ray production? ___ nm. Calculate the percentage of Emitted relative to Generated (red divided by blue as percent). _____ Is this more, less, or the same as for the case of pure Si above? ____
Please give a guess at why this might be:

Now, we also have O ka here. Calculate the percentage of Emitted relative to Generated (red divided by blue as percent). _____ This number should be significantly different than that for Si Ka.
Please give a reason why:

III. Thin Film Simulations

The instructions are pretty much the same as for the above case, the only difference being that in the first setup, Edit Layers, you click the Multi Layer rather than Grain Boundary button.

Consider a half micron (500 nm) of Ni (density 8.9) on a SiO2 substrate (density 2.62).

1. Start at 20 kV. Do the electrons penetrate the substrate? ___Are x-rays being produced from both the top film and the substrate? ___ Observe the different behavior of Ni K and L xrays.

Using the phi-rho-Z plots, fill in the blanks, using the values given in the upper right of each plot (Blue=Generated or "non-absorbed; Red=Detected or "absorbed"; % Detected = red/blue)

Ni K generated ____ Detected ____ % Detected____
Ni L generated ____ Detected ____ % Detected____
Si K generated ____ Detected ____ % Detected____
O K generated ____ Detected ____ % Detected____

2. Drop again to 10 kV. Same questions. Do the electrons penetrate the substrate? ___Are x-rays being produced from both the top film and the substrate? ___

Ni K generated ____ Detected ____ % Detected____
Ni L generated ____ Detected ____ % Detected____
Si K generated ____ Detected ____ % Detected____
O K generated ____ Detected ____ % Detected____

3. Drop now to 8 kV. Do the electrons penetrate the substrate? ___Are x-rays being produced from both the top film and the substrate? ___

Ni K generated ____ Detected ____ % Detected____
Ni L generated ____ Detected ____ % Detected____
Si K generated ____ Detected ____ % Detected____
O K generated ____ Detected ____ % Detected____

Why are there no Ni K xrays at 8 kV?
_____
What patterns do you see here? _____
_____
_____

Consider now the case of a half micron of SiO2 atop Ni, at 10 kV. Why is the result so different from the case above where Ni is atop SiO2 at 10 kV?

Write/attach a short summary paragraph discussing what you have learned about electron scattering and x-ray production/x-ray emission, comparing/contrasting homogeneous versus non-homogeneous samples.

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