

Geology 777 – Monte Carlo Exercise I

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 that 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 electrons come from the same region? What about secondary electrons?

For the hard core....Consider looking at the 1991 *Scanning Microscopy* paper by David Joy (**An Introduction to MC Simulations**; go to class website and navigate to folder with papers, then to specific Journal) to get a better general understanding of what these programs are modeling.

This week you will run electron-solid Monte Carlo simulations with the CASINO (Windows)¹ application. It can be downloaded from its homepage www.gel.usherbrooke.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). **Download only the v2.48 version!** (Not the newer version v3.2 which is a 3d simulation which no one here has yet figured out how to run!) Unzip it and be sure to run it from a folder/directory which contains the “int” folder at the same level as the .exe file.

Note: there is an article in 2007 *Scanning* on this program which you might consider looking at (posted on the class website): Drouin et al, 2007, CASINO V2.42 - A fast and easy-to-use modeling tool for scanning electron microscopy and microanalysis users.

The program models both the electron scattering and the X-ray production by those electrons, and is useful for determining what kind of accelerating voltage must be used to keep the electrons and the x-rays within the top layer. Remember that it takes more energy to produce an X-ray than the actual energy of said X-ray (ex: Si-K α X-ray = 1.74 keV, Si K absorption edge = 1.84 keV)

It is set up to simulate both bulk specimens, plus a thin films (could be more than one) over a substrate

You have 3 problems to run for your assignment: Compare the electron scattering and x-ray generation in (1) Si and (2) Au solids. (3) Look at a thin film.

Background: Using resources² at hand, fill in the blanks: _____ can 15 keV beam excite this line?
Si Ka characteristic energy _____keV minimum excitation (edge) energy for this _____ keV Y N
Au Ka characteristic energy _____keV minimum excitation (edge) energy for this _____ keV Y N
Au La characteristic energy _____keV minimum excitation (edge) energy for this _____ keV Y N
Au Ma characteristic energy _____ keV minimum excitation (edge) energy for this _____keV Y N

I. Bulk Sample of Si metal

Instructions for bulk samples:

1. Run Casino v. 2.48

¹ If you use a Mac computer, you will either need to use a Windows emulation program on it, or find a windows computer for this and many of the other programs you will need to run for this class. There is a standalone windows computer in Weeks 306 which you may use.

² Tables 14.6, 14.7, 14.8 from Goldstein et al, distributed first day of class. Or relevant tables in Orange X-ray book handed out Class 1.

2. File-> New, automatically opens Edit Layers dialog box, click Add Layer, then select the Undefined (=Substrate) and for Composition, type in Si (case sensitive) and it should put in the proper density for the metal (note: it will NOT give the correct density for non-metals, and you will need to manually enter correct values). 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:

- Define the accelerating voltage (we only use a constant one): change from 1 to **15** kV,
- Number of electrons to simulate, default is 200, but really gives poor statistics. (Set to **2000**; you will want to run 10 thousand or more runs.)
- Beam radius (nm): default is 10 nm which might be for a low current (50 pA) field emission SEM. For a more realistic beam size for a tungsten filament at 20 nA, use a 250 nm diameter (=125 nm radius) beam
- Click Next --> to go to next setup box.

4. Distributions Dialog box. Generally leave this alone. Click Next --> to go 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 **2000**. Leave rest alone. Click Next -->

6. Select Physics Model; here you can "peek 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.

8. 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> 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), or with the auto adjust button. Wait for the simulation to finish.

Questions: what is the BSE coefficient (as fraction/decimal)? _____ Having scaled the display, eyeball the maximum dimensions of the inelastically scattered electrons (blue ones), not using any single outlier, but a value ~90% of the farthest electron (straight line). If the electron trajectories got to the edges, then rescale the display:
View→Adjust Scale→Double the x and y values

Electron range in Z _____ nm Radial electron range in X (or Y) _____ nm (Not Diameter)

9. 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.

What is "electron range"? While used much, the definition is not always easily found in general books on SEM and EPMA. One definition I found, in the orange X-ray Data Booklet, is "The electron range is a measure of the straight-line penetration distance of electrons in a solid", where they cite Everhart and Hoff, J. Appl. Phys, 42, 5837 (1971). You will see that for many materials there is a difference between furthest in Z (depth) vs furthest in X or Y (radial distance)

Open each option up one by one.

10. 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 interpret 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. What is the surface radius? _____um Diameter (2 x radius)? _____um
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 (the 25% line, in green), 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? _____

11. X-Ray -- these are the Phi Rho-Z³ (PRZ) 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 x-rays suffer absorption (IN THE SPECIMEN!) and only those near the surface escape "untouched".

Note that here and in virtually all samples, the maximum intensity (y axis) is at some short distance from the surface (recall depth is plotted to the right on X-axis). This is because maximum lateral scattering occurs below, not at, the surface. At what depth in Si does maximum lateral scattering occur? _____ nm

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). _____

12. 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.

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

³ Refers to x-ray generation as a function of depth in the sample: Phi=generation; Rho=density; Z=depth.

II. Change the target to Au:

Au Z=79 density= 19.5 Now, run Au in the same way as you did Si before.
How does the electron range compare between Au and Si, for the same beam energy?

Look at the X-ray phi-rho Z plot for Au La. : At what approx maximum depth (99%) of Au La x-ray production? _____ nm. Calculate the percentage of Emitted relative to Generated (red divided by blue as percent). _____

Look at the X-ray phi-rho Z plot for Au Ma. : At what approx maximum depth (99%) of Au Ma x-ray production? _____ nm. Calculate the percentage of Emitted relative to Generated (red divided by blue as percent). _____

Compare (1) maximum depth (~range) of Au La vs Au Ma x-ray production; (2) Emitted vs Generated percent for Au La vs Au Ma x-rays. Explain the behavior.

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 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? _____

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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