Geology 777 – CASINO 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 elections come from the same region? What about secondary electrons?

This week you will run electron-solid Monte Carlo simulations with the CASINO (<u>Windows</u>) ¹application. It can be downloaded from its homesite <u>www.gel.usherbrooke.ca/casino/</u>. 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 v2.51 version!** (Not the newer version v3.3 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.

This week we will focus on electrons and how they scatter. Next week we will focus on the X-rays generated.

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

We start by comparing the electron scattering in (1) Si and (2) Au solids.

I. Bulk Sample of Si metal

Instructions for bulk samples:

1. Run Casino v. 2.451

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:

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

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.

b. Number of electrons to simulate, default is 200, but really gives poor statistics. (Set to 5000; you will want to run 10 thousand or more runs when you are really interested in better graphics for publication.)

c. 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

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.

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 \rightarrow Adjust Scale \rightarrow Double the x and y values

Electron depth in _____ um Maximum electron diameter _____ in um

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 we will look at next week). 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.

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)

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 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. What is the surface radius? _____ um Diameter (2 x radius)? _____ um

6. Energy of Surface Radius of BE--low relevance here

II. Change the target to Au:

Au Z=79 density= 19.5 Now, run Au in the same way as you did Si before.

BSE coefficient_____ Electron depth in _____ um Maximum electron diameter _____ in nm How does the electron range compare between Au and Si, for the same beam energy?

III. In the above experiment, your accelerating voltage was 15,000 volts (15 kV). Now rerun the two materials at 30 kV, and then at 7 kV.

Make a table similar to template below, for each material, at 7, 15 and 30 kV (a) electron scattering depth, (b) electron scattering diameter, BSE coefficient. Estimate the depths and diameters to nearest tenth of a micron (e.g. 575 nm = 0.6 micron)

| | 7 kV | 15 kV | 30 kV |
|----------|------|-------|-------|
| Depth | | | |
| Diameter | | | |
| BSE coef | | | |

Write/attach a short summary paragraph discussing the effects that composition (usually considered at atomic number effect, and beam voltage) on the extent of scattering with solids.

Version history 9/11/2007 9/26/07 9/8/08 10/3/08 9/24/09 10/8/10 1/30/12 2/20/12 1/18/13 1/25/13 1/26/14 9/13/16 9/16/16 1/21/18 2/9/18 2/24/18