Geology 777 – CASINO Exercise 2 – X-ray Generation

Purpose

     Last week you started to use CASINO to model electron scattering. We will now use CASINO for some modeling of X-ray generation. Since you turned in your CASINO Exercise 1 homework, I will repeat some of the material ONLY for background. But only answer the questions related to the X-ray theme.

     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 is takes more energy to produce an X-ray than the actual energy of said X-ray (ex: Si-Kα X-ray = 1.74 keV, Si K absorption edge = 1.84 keV)

     You have 2 problems to run for your assignment: Compare the x-ray generation in (1) Si and (2) Au solids.

Background: Using resources[1] 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 chacteristic energy _____keV   minimum excitation (edge) energy for this _____ keV   Y N
Au La chacteristic energy _____keV   minimum excitation (edge) energy for this _____ keV   Y N
Au Ma chacteristic 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. 2.51

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,
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 -->

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[1] Tables 14.6, 14.7, 14.8 from Goldstein et al, distributed first day of class. Or relevant tables in links given on class web page under heading "X-ray details and data", half way down the page.

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➔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.
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 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 volumes from which specific X-rays can be generated, as well as 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 _____

For background context; do not answer

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-Z^2 (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

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.

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

Write/attach a short summary paragraph discussing what you have learned about x-ray production/x-ray emission.