

Up to now we have been using Monte Carlo simulations mainly to examine the spatial extent of high energy electron scattering in materials. Some of the previous software also included simulations of the x-ray generation within a material and estimates of x-ray absorption within the sample (“matrix effect”), known as the phi rho Z curves. (Much more on that later in the course.)

One of the students of Raynald Gauvin (CASINO originator), Hendrix Demers, created a windows simulation of X-ray spectra. The program is still in development and part of using the program is to identify ways to improve it—so if something doesn’t work, let me know!

A program like this (and CASINO phi rho Z ability) is valuable not only for learning basic concepts but also in the real-world lab. Since these programs are based upon the physics of the processes (understood more-or-less pretty well)¹ we can compare real life data with the simulated data, and troubleshoot faulty hardware – or faulty software.

This week we will first go through some step-by-step instructions to learn about the features of Win X-ray, and then run some simulations that allow us to simulate some of the data we acquired in the EDS lab this week.

You can download Win X-ray from the official site: montecarlomodeling.mcgill.ca (probably best to get it there as that should be the latest version, vs whatever I have sitting on the class web page.) The most recent version is 1.3.1 (as of 9/2009)

1- Demonstration of Win X-Ray for simple case of Cu at 10 kV

Open the Win X-Ray program

Chose File ->New

Now in Option Simulation window

Set Incident Energy Start to 10 kV

Set the number of electron trajectories to 1000

Defaults ok: eg. Beam Diameter 10 nm.

Set Beam Current to 2e-8 A (=20 nA)

Check X-Ray Compute and Compute Characteristic, and Compute Background

Change TOA (take off angle) appropriate one for your SEM or EMP,

e.g. here change to 40 and Theta (=90-TOA) X-ray to 50

Click Next button

Now in Option Specimen window

Click on Set Element for All Regions button for defining target composition, here only 1 element

Now in Option element for region 1 window:

Change the atomic number Z to 29, or Symbol to Cu (Must capitalize 1st letter!)

NOTE: Wt fraction total must =1, so if changing to multi-elements back to single element, make sure the weight fraction always is set correctly. Otherwise you cannot proceed

Click Ok button (leave Option element for the region 1 window)

Back to Option Specimen window

Click Next

Now in Option X-ray window

¹ Though in some cases are/could be based upon empirical data, so similar samples should give good results regardless of how well the physics is understood.

Set time in seconds to how long to run: start with 100 sec; Window should be 8 micron Be
 Click Next button

Now in Advanced Option window
 Ignore for now, click Next button

Now in Physics Model window
 Ignore for now, click Next button

Now in Result General Option window: irrelevant for you here, but here is the meaning
 [Save result in File = Automatic (will automatically save all files in a folder in the Program folder); Manual means turn off because you want to manually write down the numbers]
 Click Next button

Now in Result Trajectory Option window
 Check box to see a small number (e.g. 200) trajectories while the x-rays are being
 Click Next button

Now in Result Distribution Option window
 Generally ok to accept the default values here
 Click Finish ... and it is running though nothing appears to be happening: look at the bottom bar

Wait for the end of the simulation: bottom menu bar shows % progress, elapsed and remaining time.
 Last number (n) is the backscattered coefficient that is constantly being updated.
 Data now ready when the small “10 keV” indicator in the upper column is no longer greyed out.
 Click on + to expand the tree view
 Click on the trajectory +
 Click on the interaction volume and adjust the new windows as you wish
 Move the mouse over the picture to find the max depth and radial dx (shown in bottom of image)

Change the X-Z Plane to X-Y Plane by clicking the X-Z window immediately above, then X-Y
 Click on BSE
 Take some of the choices, see how much more freedom you have to read specific things, such as distances, just by moving the cursor over the image, with readout on the bottom bar.

Click on the X-Ray +
 Click on the PRZ Curves +, then particular element (Cu), then particular line (e.g., Ka1, Lb1)
 → Note that x-ray intensity vs depth (Z, on the horizontal axis), showing the generated (red) and emitted (green) distributions, easiest seen for the L lines.
 Click on Spectrum to show the complete spectrum with the effect of the detector
 Click on the Y Axis Log
 Check and uncheck Background, Characteristic, and Total
 Move the mouse to read energy and intensity at the cursor.
 Without Y log scale checked, zoom on the K-Lines by left click + move down and right with the mouse to select the zoom region.
 To reset the view left-click + move up and left with the mouse.

Now click Intensity: I Detect is the integrated Peak minus Background counts for each peak;
 Note the INTENSITY value for Cu Ka1: _____ and Cu Ka2: _____
 Add them together _____ (call it “a”)

Now click on “lines”, Cu, Ka1: here you see a modeled characteristic peak (yellow), continuum (green) and “total” P+B in red. Note that its center is not the same as the yellow peak. This is an intentional undocumented feature and the red peak is total in more than one sense of the word. It is a weighed total of the Cu Ka1 and Ka2 peaks. Note the value for Total (red) Cu Ka1 _____ (call this “b”)--this is a much smaller number than “a” because it is the single channel number.

One of the benefits of EDS over WDS is that the computer will integrate ALL the xrays in the peak curve – giving a higher number than just in the one single channel that is the theoretical peak position.

The take home message here should be that (1) background needs to be subtracted (as when doing quantitative analysis) and (2) if you can integrate under the peak [easy in EDS!], you will have a lot more counts to improve your statistics (precision) and also (3) that Ka1 and Ka2 peaks are very close and in EDS you cannot distinguish. The reason he shows both Ka1 and Ka2 is that BOTH can be modeled in his Monte Carlo process. Why is there Ka1 and Ka2? Dig into the references (slide from 2nd class with “onion skin” families of x-rays, also in Goldstein) and tell me precisely what **two** shells are involved with Ka1 _____ and with Ka2 _____.

2- L lines from Ag

Select in the menu Option->Option Specimen

Click on Set Element for All Regions button

Change the atomic number Z to 47, or Symbol to Ag

Click Ok button

Click on Simulation->Run or the green “play” button

After it is done, click Intensity and write down the energies for these 4 characteristic lines:

La _____ keV Lb1 _____ keV Lb2 _____ keV Lg _____ keV

Now look at the Spectrum for the L-lines – Note the 4 distinctive L lines (and he is leaving out 2 others that he should show to be totally accurate, 2 lines that would appear to the LEFT of the La, the L 1 (that’s L L) and L n (L N) peaks.

Compare the relative heights of the characteristic peaks (red)

La _____ Lb1 _____ Lb2 _____ Lg _____

3- Effect of changing accelerating voltage on Cu La/Ka ratio

Here we will acquire Cu La and Cu Ka1,2 data at 10, 15 and 20 keV.

Measure values Cu La, Cu Ka1, Cu Ka2, in Intensities. Sum Cu Ka1 and Ka2, as these two peaks are very close and EDS sees both as one single peak.

Run at 10, then 15, then 20 keV

Fill in the table below

kV	La	Ka1	Ka2	Ka1+2=Ka	La/Ka
10					
15					
20					

Explain **why** La/Ka has a distinctive trend with increasing accelerating voltage

4- Effect of carbon build up (contamination) on detector window for problem as #3 above

Here we can examine the effect of having a thin contaminant layer on the window of the EDS detector.

Run at 10 keV on Cu.

In Option X-ray, in Contaminant Thickness, set Carbon to 0.1 micron, and then 1.0 micron.

Fill in the table below.

kV	La	Ka1	Ka2	Ka1+2=Ka	La/Ka
0.1 um carbon					
1 um carbon					

What is the effect on Cu Ka counts?

On Cu La?

Any difference?

Why?

Why would it be dangerous to attempt to do “EDS Standardless Analysis” (using stored intensity files, gathered years before) for Cu using the La x-ray line?

What about for measuring even lighter elements (e.g. Oxygen)?

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