**Geology 777 Exercise 4: Win X-ray-2 10/4/09 Name _____**

G777 Exercise 4: Using Win X-ray to simulate some more complicated spectra

This week your goal will be to continue using the WinX-ray program and create several spectra, and then look at these spectra to get a more advanced understanding about the process of X-ray generation and detection. Since the program is grounded in the basic physics, we are essentially doing real experiments, albeit with "perfect" detectors which do not have Si-escape peaks, sum peaks, nor Si-internal fluorescence peaks.

1. Simulate an EDS spectrum of a 5-element material that is (by weight) 20% Na, 20% Si, 20% Ca, 20% Fe and 20% Se (enter data as fractions, e.g. 0.2). Use 500 simulated trajectories. Operate with E0 of 15 kV. This is to simulate the intensities with the good-old Si-Li detector. Use all the other settings the same as you did last week (attached appendix).

You should see more than 5 peaks in the spectrum, right? Click under X-ray → Spectrum and count the peaks you see…Hint: Y axis Log helps. ____

OK, now click on Intensity under X-ray where there is a table of all the lines it is claiming exist for this sample… how many lines does it say? ___

Why the difference?

Now make a list of the observed element lines, IN INCREASING ENERGY (eV) order. Show only lines which can be pass thru the Be window (i.e. 500 eV). Combine vy close lines (Ka1+2) into 1.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Energy (ev) | | | | | | | | | | |
| Element | | | | | | | | | | |
| Line | | | | | | | | | | |

Fill in the table below for the 5 elements and their Ka values. Sum together the element Ka1 and Ka2 intensities into one value. NB. Use the Intensity tab, NOT the Lines tab, to get these numbers.

| Element | Atomic No. | Charact. Energy (keV) | Binding Energy (keV) | Detected Intensity (Ka1+2) | Overvoltage |
|---|---|---|---|---|---|
| Na | | | | | |
| Si | | | | | |
| Ca | | | | | |
| Fe | | | | | |
| Se | | | | | |

Each element is present in the same mass abundance. Are the x-ray intensities likewise the same? ____
If not, discuss what might be involved in affecting the detected intensities.

2. We want to create EDS spectra for 3 binary alloys of Fe with either Ni, Mn or Cr. All at 20 kV. Here are the exact compositions: WEIGHT not ATOMIC:
(1) Fe 50 wt%, Ni 50 wt%
(2) Fe 50 wt%, Mn 50 wt%
(3) Fe 50 wt%, Cr 50 wt%

Simulate each spectrum, using 500 simulations. Fill in the table:

| Alloy | Fe wt fraction | Fe Ka1+2 = I(alloy) | I(alloy)/I(pure Fe) |
|---|---|---|---|
| Fe-Ni | 0.5 | | |
| Fe-Mn | 0.5 | | |
| Fe-Cr | 0.5 | | |

Now do a simulation for pure Fe. Use this as the denominator for the 4$^{th}$ column above. As we shall see soon, using some reference material (a standard) to compare counts from an unknown, is a very useful technique.

Is the Fe Ka(1+2) intensity the same in all 3 alloys?

If not, what might be involved in the differences?

Filling in the table below may help. Think about x-rays as not only effects (from electron attack) but also as causes with their own effects…

| Element | Characteristic Ka energy | Binding energy (K shell) |
|---|---|---|
| Fe | | |
| Cr | | |
| Mn | | |
| Ni | | |

Discuss your conclusions.

general instructions from last week

***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
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")

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