Geoscience 777   Exercise 5: DTSA-II 2nd 2/23/2019   Name _____

Using DTSA-II to simulate some more complicated spectra

This week your goal will be to continue using the DTSA-II 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. Select the Oxford AZtect SDD detector you created last week.
2. Inside the Simulation Alien, Configure the Sample composition, and create a "MagicStuff" 5-element material that is (by 'mass fraction') 20% Na, 20% Si, 20% Ca, 20% Fe and 20% Se (enter data as %, i.e. 20). Give it a density of 5 g/cm^3. **Set instrument configuration to 15 kV and all other settings same as last week. This is to simulate the intensities with the Oxford AZtect SDD detector. Use all the other settings the same as you did last week.**

You should see NINE (or maybe TEN?) peaks in the spectrum.

Why are there more than 5 peaks?

Now make a list of the <u>observed</u> peaks, IN INCREASING ENERGY (eV) order. Show only lines which can be pass thru the Be window (i.e. 500 eV). Consider close lines, e.g. Ka1,2, as ONE . (You may not need all the boxes.)

Energy (eV)													
Element													
Line													

Fill in the table below for the 5 elements and their Ka values. Consider close lines (e.g. Ka1,2) intensity as one value. Use class notes for translating IUPAC notation (e.g. L3-M4,5) to Siegbahn (La1,2). For background intensity, you just need to estimate it roughly, averaging ("eyeball") it. Remember the definition for Overvoltage: E0 divided by binding energy.

Element	Atomic No.	Charact. Energy (keV)	Binding Energy (keV)	Peak Intensity (Ka1,2)	Background Intensity	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.

3. 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. For density, use a linear (mass) combination of the pure element densities.
(1) Fe 50 wt%, Ni 50 wt%
(2) Fe 50 wt%, Mn 50 wt%
(3) Fe 50 wt%, Cr 50 wt%

Simulate each alloy spectrum. Fill in the table. Measure Fe Ka peak count intensity. Estimate background as best you can. Let I = Pk-Bkg of the element. This means peak counts minus background counts.
Now do a simulation for pure Fe. Measure Peak and Bkg counts. Calculate Peak minus Bkg. Use this as the denominator for the 4th column below. As we shall see soon, using some reference material (a standard) to compare counts from an unknown, is a very useful technique. **The 4th column is what is known as the K-ratio, and is the basic unit of electron microprobe quantitative analysis**

Alloy Density	Fe wt fraction	Fe Ka Peak Counts	Fe Ka Bkg Cts	I(alloy)/I(pure Fe)
Fe-Ni	0.5			
Fe-Mn	0.5			
Fe-Cr	0.5			

Is the Fe Ka intensity the same in all 3 alloys?

If not, what might be involved in the differences?

Fill in the table below.. Think about x-rays as not only effects (from electron "attack" but also as causes with their own effects ("X-ray attack")

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

Discuss your conclusions in a paragraph on a separate piece of paper, paying particular attention to the K-ratios for Fe-Ni, Fe-Mn, and Fe-Cr and the relation between the maximum and minimum values and the significance of the characteristic and binding energies for the alloys with max and min K-ratios.

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