

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 Be window (8 um) Si-Li detector you created last week.
2. 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. Set instrument configuration to 15 kV and all other settings same as last week. 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.

You should see more than 5 peaks in the spectrum, right? Hint: Y ("ordinate") axis as Log might help.

Why are there more than 5 peaks?

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 vey close lines Ka1,2 into 1. (You may not need all the boxes.)

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 as one value.

Element	Atomic No.	Charact. Energy (keV)	Binding Energy (keV)	Peak Intensity (Ka1,2)	Bkg	Overtoltage
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. 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 spectrum. Fill in the table. Measure Bkg to left of peak. Let $I = Pk - bkg$ of the element

Alloy	density	Fe wt fraction	Fe Ka _{1,2}	Background	$I(\text{alloy})/I(\text{pure Fe})$
Fe-Ni		0.5			
Fe-Mn		0.5			
Fe-Cr		0.5			

Now do a simulation for pure Fe. Measure Peak and Bkg. Calculate $Pk - Bkg$. Use this as the denominator for the 4th column above. 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.

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.

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