Name _____   Week of Feb 19, 2019

Exercise 4: Getting familiar with DTSA II (Desktop Spectrum Analyzer)

PART I-Installing DTSA II   What is DTSA II?
        DTSA II is a research-grade program that (1) can be used to process raw x-ray data (i.e. spectra or K-ratios) generated by x-ray spectrometers and also (2) allows generation of synthetic X-ray spectra. We will be using it in the second capacity.
        Four short articles plus one long power point slide show about DTSA are archived on the class website: http://www.geology.wisc.edu/~johnf/g777/DTSA.html
        Go ahead and download all 5 items to your computer. Open up and read *Ritchie, 2011 (January), Getting started with NIST DTSA-II.*

Installing DTSA II:
Go to the following site:

https://cstl.nist.gov/div837/837.02/epq/dtsa2/index.html

Brand new in 2019 -- You Tube videos

Read the Introduction. Then click INSTALLATION

Below 'DOWNLOAD' click the DTSA-II link and follow the instructions detailed under the 'INSTALLATION' section (same webpage).

   • DTSA-II Kelvin (multiplatform Java installer)

Before you start working with DTSA II you must create a detector with the configuration of the detector used in your lab. Below we give the parameters for the Oxford Aztec SDD detector. If you have access to an EDS in another lab, you could create (in a separate folder) that detector.

The steps to do this are as follows (Note: the screen shots are for our previous EDS system):

Click File (Far left DTSA button)→Preferences→Instruments and Detectors→ADD→Name instrument with Detector (Here: G777 Aztec simulator)→ADD SDD Detector→
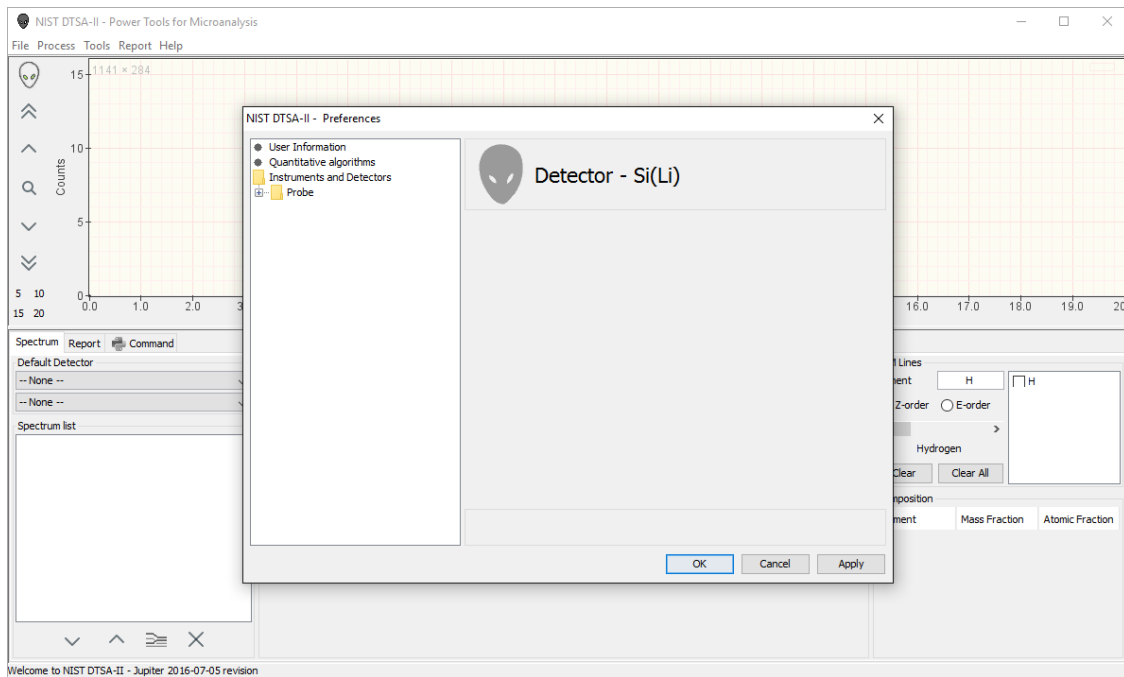
Set detector parameters as follows→Click OK when finished:

- Under STATUS→Verify that 'Enable detector' is checked
- NAME→Weeks 302 SDD
- WINDOW→Moxtek AP 3.3

If necessary, scroll down with right scroll bar to get to Position, etc

Under POSITION:

- Elevation angle→35.0
- Azimuthal angle→0.0
- Optimal working distance→10 mm
- Sample-to-detector distance→35 mm

Under CRYSTAL PARAMETERS:

- Detector area: 10 mm^2
- Gold layer: 0 nm
- Aluminun layer: 0 nm
- Nickel layer: 0 nm
- Dead layer: 0.08 um
- Thickness: 0.45 mm
  (Please check and verify that these settings are actually saved, for debugging this program. If not saved, you still can simulate fairly realistic spectra. There may be a bug here.
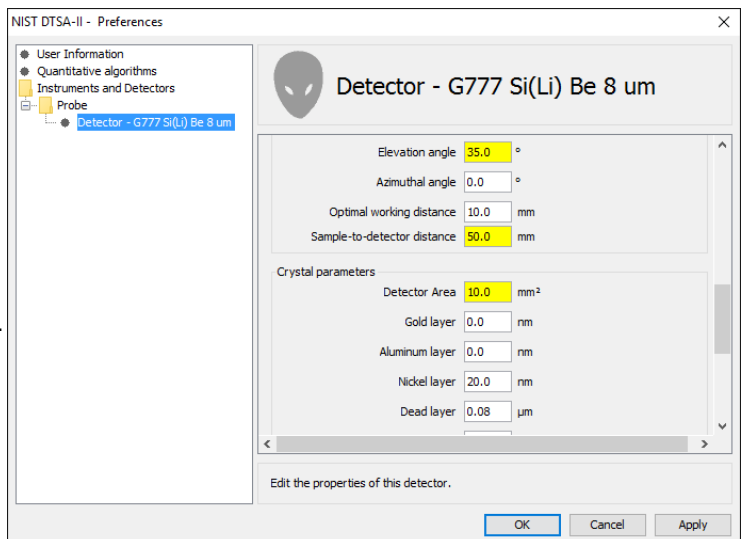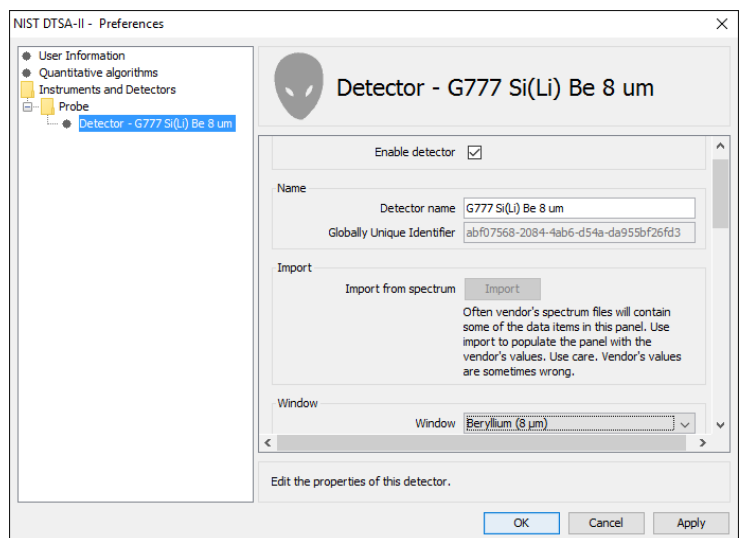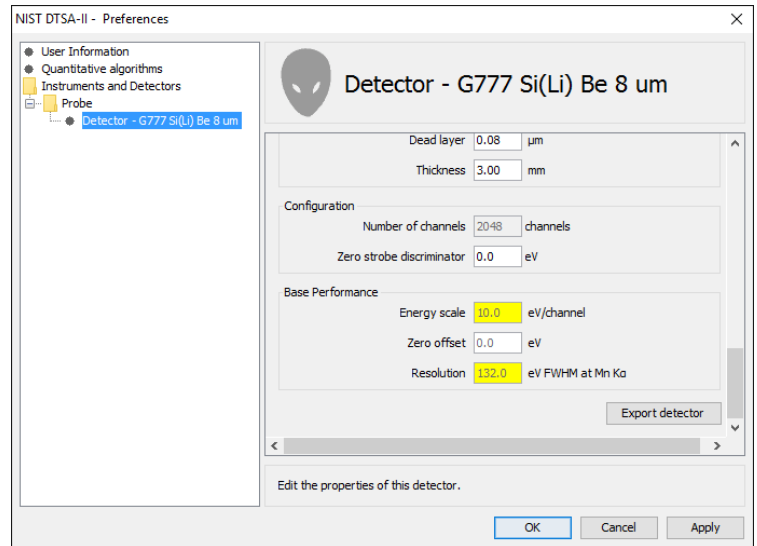
Under CONFIGURATION:
- Zero strobe discriminator→0.0 eV

Under Base Performance
- Resolution: 129 (@Mn Ka)

The click Apply, and OK to exit

PART II- Simulating Spectra

Go to the following link and select SIMULATION (left hand side MENU) or details on simulating spectra and the difference between a Monte Carlo simulation and Analytical simulation. Carefully read through the one page tutorial.
https://www.cstl.nist.gov/div837/837.02/epq/dtsa2/index.html

Let's perform a simple **analytical** simulation (simpler and quicker than Monte Carlo):
1. Cu at 30 keV
2. Cu at 20 keV
3. Cu at 10 keV
4. Cu at 5 keV

To do this:
- Go to TOOLS→SIMULATION ALIEN→Analytical model of a bulk homogeneous material→Next
- Under Materials and Scale click EDIT, a window like the one to the right will show up:
- Type Copper or Cu and click on the magnifying glass icon→ Note that the density did not change. You must insert the density. Look it up in a book or google it. Enter 8.9. →Click OK. (You are creating a database).
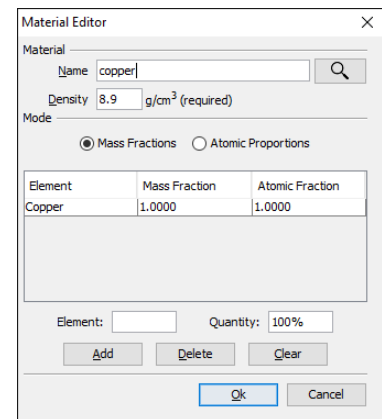
The CONFIGURE SAMPLE window will show up again, Copper will appear as bulk material→NEXT→Change the Beam energy to the desired keV (start with 30 keV) Probe dose=60. Incident angle =0 (means the beam is at 90° relative to sample surface)
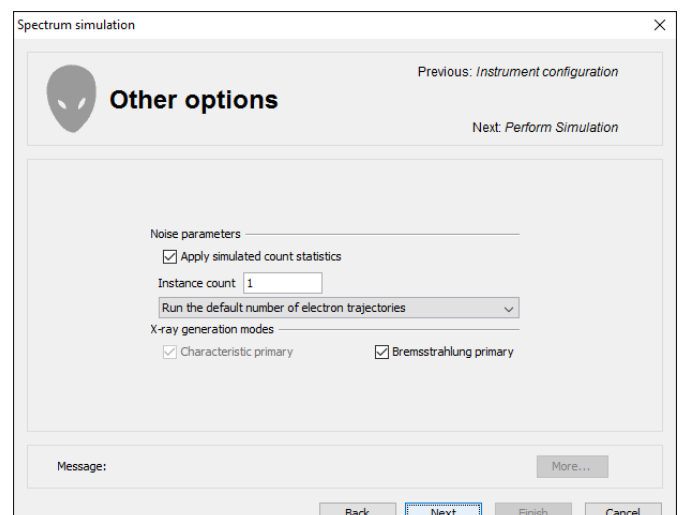
→NEXT

This window will show up:

1. Check 'Apply simulated count statistics'
2. Instance count= 1 (just one simulation of the requested model; no reason to do this unless Monte Carlo)
3. Under 'Extended output' select

'Run the default number of trajectories' (?#?)

4. Characteristic and Bremsstrahlung checked
5. Click NEXT→FINISH
6. (You will repeat this later for different keV settings, but now just answer these questions)

Questions:

1. How many peaks are there in the 30 keV spectrum? ___ And this is for one element, right?

2. Now write down the energy for the center channel of each peak:

3. Instructions: Start with **tall peak about 8 keV**: double click just to left of it, then drag across peak to right side and release, area now in yellow. Right click over area and select "zoom to region". In the KLM Lines box to right, type in "Cu" in element box (+ hit enter). Now what two lines (see appendix on last page) show up (hint: K and some Greek letter that sounds like A)? And what are the energies? And what are the counts? To get this info, double click on the characteristic line and you have 10 seconds to read and write down the info box before it vanishes into NIST space (you can right click, copy and paste if you want).

    Line   Energy   Peak (channel) counts
    ____   _____keV   _____

    ____   _____keV   _____

4. Now do the same for the small peak to the right of this peak. However, you have to undo the current peak and go back to the original spectrum. Easy to do by clicking "Nicholas" the Green Alien (not green anymore since the last version). Notice there is a vertical yellow line. This is "counting" mode and you need to turn it off, and go to the "select region" mode. To do this, double click on the yellow line. What is the label (line), energy and counts in the center of this small peak?

    Line   Energy   Peak (channel) counts
    ____   _____keV   _____

5. There is ANOTHER LINE to the right, right? What does it say? _____ This is the Cu K edge energy (the minimum energy needed to break the bonds of inner shell K electrons). Now repeat the "undo" (in #4) to go back to the original spectrum (the Alien).

6. Now select the region of interest a little above 0.9 keV. Use the same procedure and fill out the blanks below

Line   Energy   Peak (channel) counts

____   _____keV _____

7. Did you expect to see so many characteristic x-ray peaks from just one element?

8.   I want you now to run this simulation at 20, then 10, then 5 keV, and make a table, recording the peak channel counts for the La and the Ka channels.

9. Plot all the data: this includes the L line you saw as well as the Ka and Kb lines. On X axis plot the keV and on Y axis plot peak counts. You should have two trends, one for the La and one for the Ka. What are the trends?

  How do you explain the different trends?

  10. If you put in a Be detector window, what would be the main difference in the spectrum?

Appendix: Line Nomenclature: Traditionally we use the Greek letters for X-ray designation, such as K alpha, although in recent times more formal nomenclature is sometimes used, the IUPAC one. You will see both used in DTSAII, so here is a brief reminder:
L alpha = L3-M4,5
K alpha = K-L2,3
K beta = K-M2,3
(where, for example M2,3 means an electron from either the M2 or the M3 shell is involved)

For your homework, just using the Greek nomenclature is OK.

Thanks for Dayi Ortiz for doing most of the work in creating this exercise! (late 2011-early 2012)   Version: 2/9/12 *1/18/13 9/13/16 2/20/18 3/17/18 2/17/19*