Developing Software for the Beam Line Control Systems

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1. INTRO TO XAS

X-ray Absorption Spectroscopy is a technique used by biologists, geologists, paleontologists, and many other scientists around the world to examine the chemical components of a particular object of interest. XAS experiments have allowed scientists to develop new drugs in the medical field, find ways to increase energy efficiency, answer questions regarding historic events, and overall has been a great use in the scientific community.

Figure 1. Full image of a beam line at the SLAC National Laboratory.

4. WHY PYTHON?

Use of *Python* to implement the Region Editor Software

Python was chosen for its rapid prototyping ability, its customary use at SSRL, and a great availability of GUI and scientific libraries. Unlike MatLAB[TM], Python is an open-source, free language and software developed in Python can be given to the users for personal use.

```
        self.inp_max_time.SetValue("%.3f" % maxt)
        self.inp_power.SetValue("%.3f" % power)
        self.inp_edge.SetValue("%.3f" % edge)

def on_btn_save( self, event ):
        #print self.region_list
        #np.savetxt('reg_file.txt',self.region_list,fmt="%s %s %s %s %s %s %s %s")
        #wx.MessageBox('Your file has been saved.', 'Info',
        #   wx.OK | wx.ICON_INFORMATION)
        dlg = wx.FileDialog(self, message="Save region data as...", defaultFile="*.rgn")
        if dlg.ShowModal() == wx.ID_OK:
                regfilepath = dlg.GetPath()
                dlg.Destroy()
        else:
                dlg.Destroy()
                return
        try: # try to open the file for writing
                rf = open(regfilepath, 'w')
        except:
                wx.MessageBox("Cannot create the region file %s" % regfilepath)
                return
        # so now the file is open
        for region in MyDialog2.region_list:
                regtype, startval, stopval, inc, points, t, maxt, power, edge = region
                print >> rf, "%s, %.3f, %.3f, %d, %.3f, %.3f, %.3f, %.3f" % (regt
        rf.close()
```

Figure 4. A snippet of the code used to develop this software.
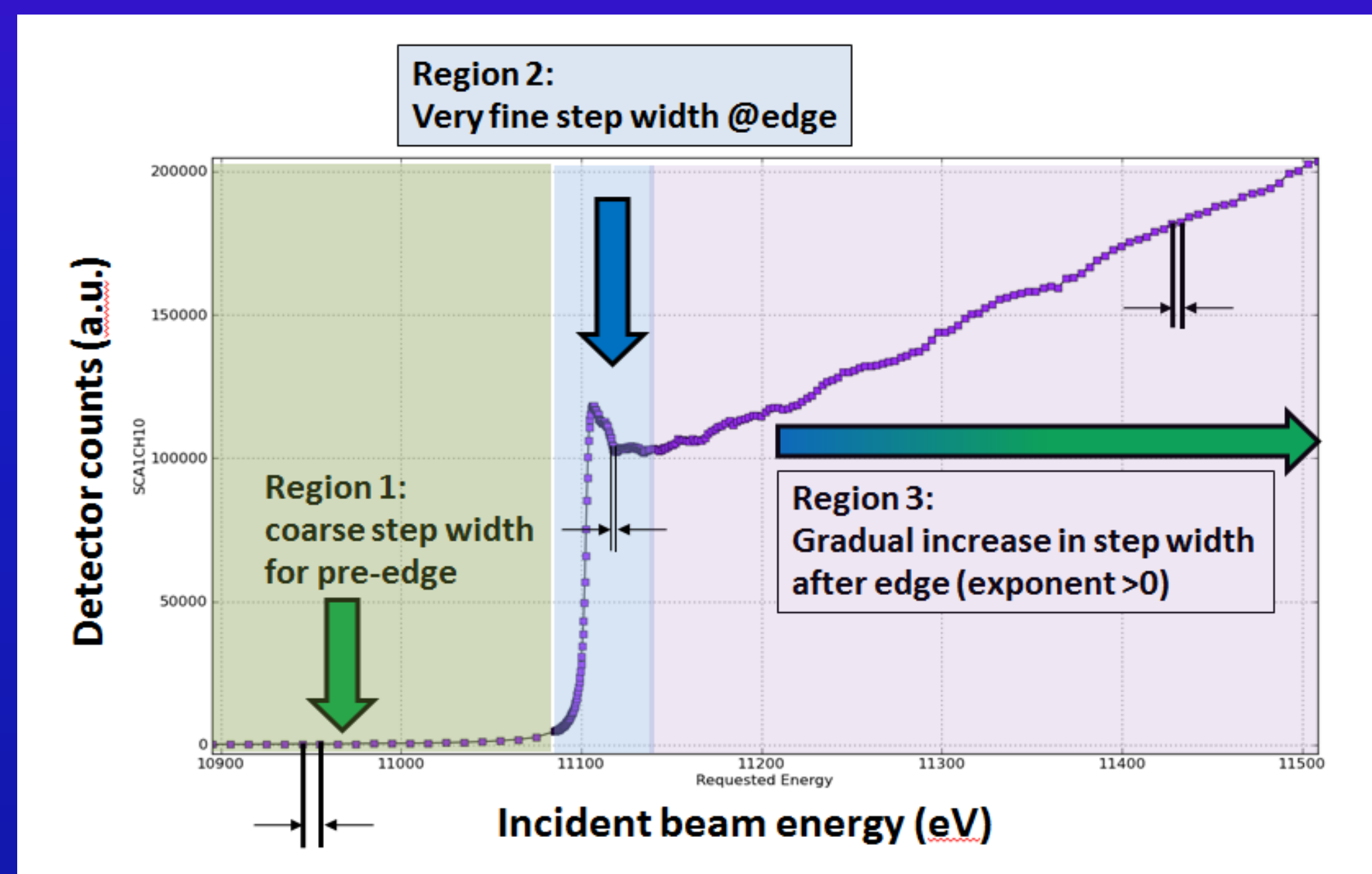
2. REGIONS

Figure 2. Graph of the spectra collected during a scan . The graph above shows that the step width is different in each region. There are more points collected in the middle region where graph depicts a jump.

In a typical XAS experiment, the incident X-ray beam energy is varied in a region close to a fundamental electronic transition of the atom(s) of interest. The data has to be collected most densely in the immediate vicinity of the transition (also called edge). XAS scans are therefore often comprised of differently dense regions where the first region is course (wide steps), the second region is dense (narrow steps), and the third region exponentially goes from dense steps to wider steps. See Figure 2.
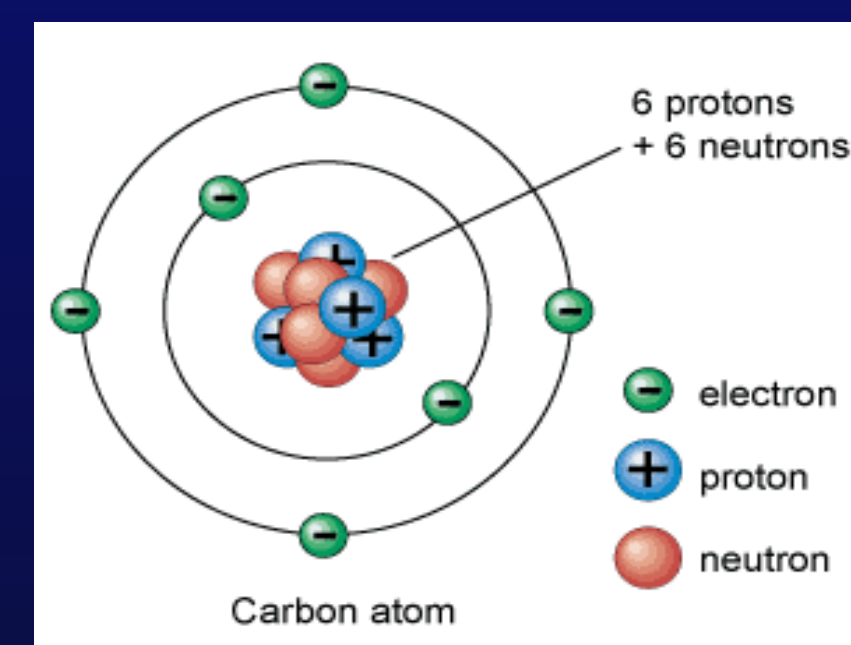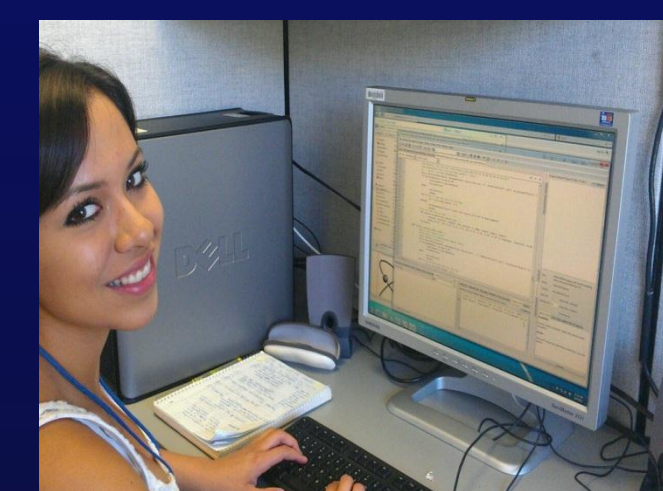

Figure 6. Image of Bohr's Model.

Image of me in my workspace.

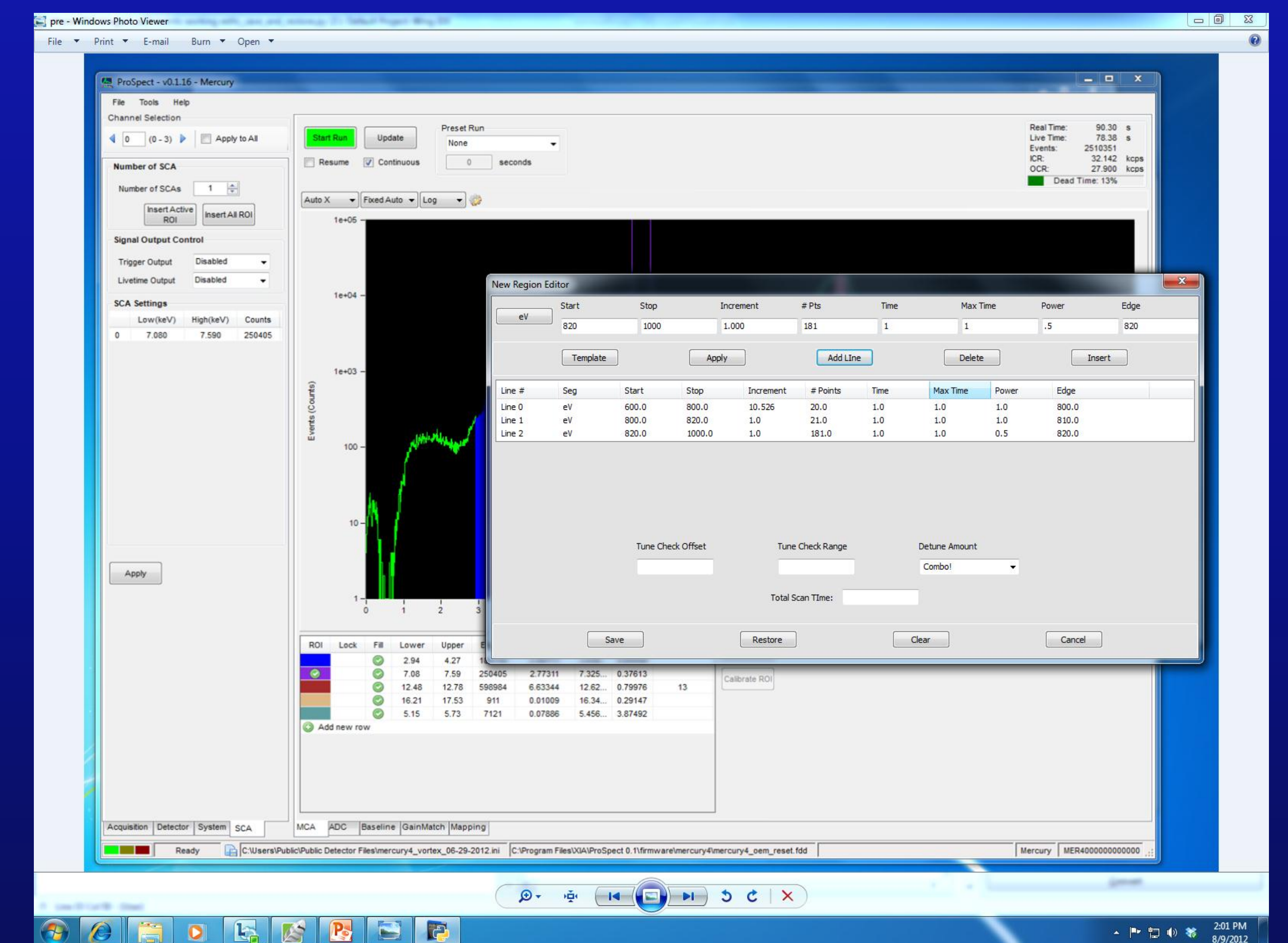Figure 7. The ring where the energy is stored for the beam lines.

3.PROBLEM/SOLUTION

The user can define how the data will be collected in each region by typing commands on the beam line console which features a command line interface (CLI). However, this is an inefficient method because it can be a lengthy, tedious, time consuming, and overall unpleasant process for those who are not computer experts. To facilitate this process we designed a graphical user interface (GUI) that has all the necessary components for the user to define each region by simply typing in textboxes and using the mouse to click on labeled buttons which execute the desired event.

Figure 5. Here is a picture of the GUI we created to help define the regions during a n XAS experiment

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