Spatially-Resolved Elemental Analysis In The Scanning Electron Microscope

Santiago Rodriguez [1]

[1]*Institut für Physik, Humboldt Universität zu Berlin, Deutschland*
Instructor: Dr. Wouter Van den Broek
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I   Abstract

In order to analyze the topography and elemental composition of samples at scales where the resolving power of conventional light is insufficient, electron microscopes use accelerated electrons as an alternative messenger particle for the process of acquiring information from a samples ultrafine structure. For this experiment, a scanning electron microscope (SEM) of the Zeiss GeminiSEM 500 series was used to capture various images of the surface of a silicon germanium sample on which small, single-crystalline islands had formed on a self-organized manner by means of liquid phase epitaxy.

The goal of this experiment is to compare the effect of different detection devices and parameters of the SEM using the SiGe sample, as well as to capture an image of the silicon germanium crystal islands and analyze the local elemental composition and distribution using the inbuilt EDX spectrometer of the SEM. The measurements in this experiment were taken at accelerating voltages of 5kV and 15kV respectively for comparative purposes, as well as at 20um, 30um and 60um aperture of the SEMs electromagnetic lens system while alternating between three of the SEMs detectors for the different experiments.

The resulting datasets and pictures show a generally better performance and consistency with the expected values at the higher accelerating voltage of 15kV, albeit at the cost of increased noise and potential sample damage. Out of the imaging detectors, the InLens detector consistently delivered sharper and less noisy images than the SE2 detector, while the EDX detector mapped considerably different elemental distributions depending on the accelerating voltage of the electron beam.

II   Working Principles of the SEM and Theory

When imaging objects on a scale similar to the wavelength of visible light $\lambda \in [380nm, 700nm]$, traditional, light-based microscopes are often limited by their diffraction limit. This limit, given by the expression $d = \frac{\lambda}{2NA}$, states the minimum distance d at which two objects surrounded by difraction rings can still be distinguished from one another at a given wavelength of the particle used for the imaging process. Because of this, light-based microscopes are often only capable of resolving objects of sizes above this diffraction limit around roughly the distance scale of $d \in [\frac{380nm}{2NA}, \frac{700nm}{2NA}]$.

In order to image smaller objects like the silicon-germanium crystals ($l \approx 100nm$) which were used as a sample in this experiment, particles of shorter wavelengths need to be used. And although it is possible to produce -as well as detect- light at shorter wavelengths than 380nm, the energy of photons at such short wavelengths -71.66keV and 124.72keV at 17.3pm and 9.94pm respectively- could heavily damage the sample. In addition, due to their short cross section, it would also be difficult to accurately generate an image with the low amount of scattering high frecuency photons. Alternative messenger particles can be utilized, however, specially if their energies remain comparatively low at shorter wavelengths, as is the case for neutrons and electrons.

Figure 1: Zeiss GeminiSEM 500 at the HU Physics Institute

Due to the difficulties in manipulating the former, as they are electrically neutral and don't interact with electromagnetic forces, the later are often used in what is known as electron microscopes (EM), which are able to manipulate the direction, focusing and intensity of these electrons using electromagnetic lenses and components analogue to their optical counterparts. Among these electron microscopes, the one which was used in this experiment is one type of EM called a scanning electron microscope (SEM) and was manufactured by Zeiss as part of its GeminiSEM 500 line of products.
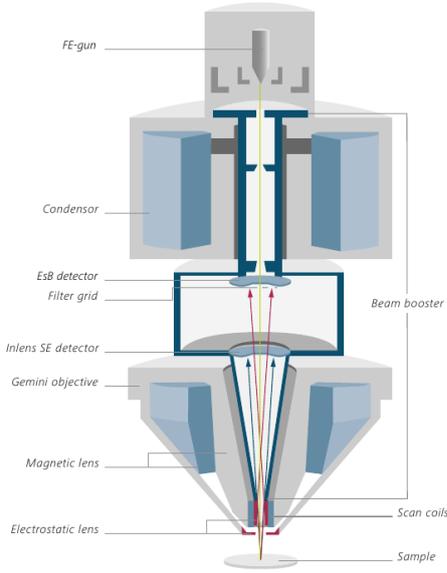
Figure 2: Inner SEM Diagram

A scanning electron microscope works by detecting and analyzing the signal of the different types of scattering processes which the electrons undergo upon hitting the sample. These can be backscattering processes, transmission processes or even inelastic processes such as ionization of atoms within the sample. According to Louis de Broglie, these interactions occur as if the electrons were behaving like a mass-carrying wave of wavelength $\lambda_e = \frac{hc}{\sqrt{eV_0(2m_oc^2+eV_0)}} \Leftrightarrow E = \sqrt{(\frac{hc}{\lambda})^2 + m_0^2c^4}$. Thus, at very short wavelengths such as 17.3pm and 9.94pm the corresponding electron beam energies would be 5keV and 15keV respectively- so energies almost one full order of magnitude lower than those of electromagnetic waves within the same spectrum. However, since these are still high energies above those required for ionization of most elements, the SEM can perform energy dispersive spectroscopy using an EDX detector -a Bruker Quantax 400 - Z30 system using a 30 mm2 Xflash 6—30 with a Peltier-cooled solid state detector- to measure the characteristic X-Rays emitted by the sample as the electron beam scans across it.
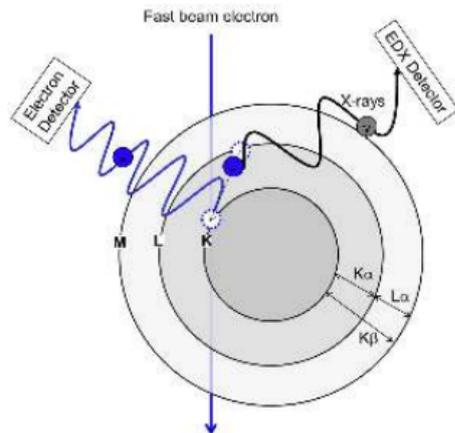

Figure 3: Illustration of an inelastic electron interaction generating a characteristic X-Ray through ionization of an electron in the K-shell of an atom within the sample

In this scenario, when electrons in the inner orbitals of an atom are removed by an inelastic colision with one of the high energy electron beams, a characteristic X-Ray is emitted once an electron from a higher energy orbit above falls to fill in the vacancy. The energies of the resulting photons in the X-Ray spectrum posess wavelengths $\lambda \propto \frac{1}{\Delta E}$ inversely proportional to the characteristic energy difference ΔE for the electron transition between the orbitals of each element. Thus by measuring the intensities of these characteristic X-Ray emissions, it is possible to measure the elemental composition of a sample; provided the signal is strong enough to stand out among the continuum X-Rays emitted by the interaction between the beam electrons and the coulomb (electric) field of the nucleus of the specimen atoms (also known as Bremsstrahlung), which in this case is a source of constant background noise for the spectrographic X-Ray measurements.

III   Imaging of the Si-Ge Islands

For the imaging of the Si-Ge islands, two of the SEM detectors were used; the InLens detector and the SE2 Everhart-Thornley detector. Both detectors are used to analyze the signal and integrate an image out of secondary electrons (SE) emmited by the sample as the electron beam scans across it as well as backscattering electrons (BSE), with the InLens detecting the first and second kind of SE electrons and the SE2 detecting backscattering electrons (BSE) alongside the second type of the aforementioned SE electrons. These SE electrons are generated at the position where the electron beams impinges on the sample surface (SE1) as well as during the course of multiple scattering interactions inside the material (SE2). Backscattering electrons (BSE) are electrons from the primary electron beam which have elastically interacted with an atomic nucleus inside the sample and scattered back towards the detector.
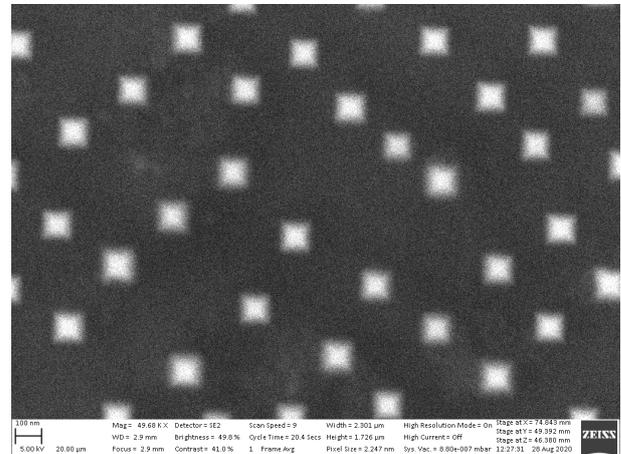

Figure 4: SE2 detector at 5kV accelerating voltage and 20um aperture

The first image was taken at $V_0 = 5kV$ accelerating voltage and $D = 20um$ aperture. With these settings,

the self organized crystalline structures on the silicon substrate become clearly recognizable, although any further details of the island themselves remain difficult to make out due to a high noise to signal ratio as well as a noticeably low contrast.
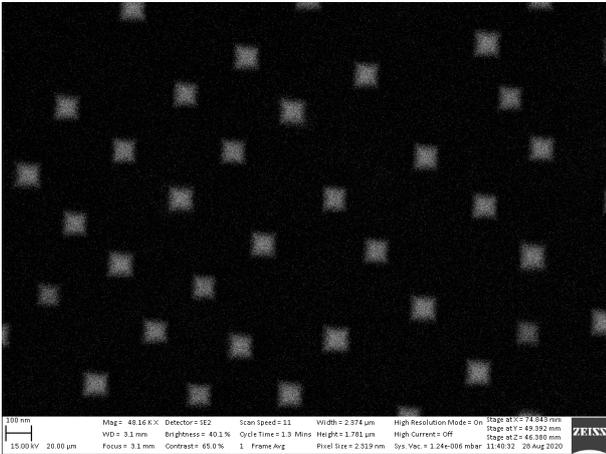

Figure 5: SE2 detector at 15kV accelerating voltage and 20um aperture

At a higher value for the accelerating voltage of $V_0 = 15kV$, the contrast of the resulting image greatly increases, as well as the sharpness. However, the details of the SiGe crystals remain largely unrecognizable, with an even higher amount of noise mostly impeding the viewing of any further information on the crystals structures within the image.
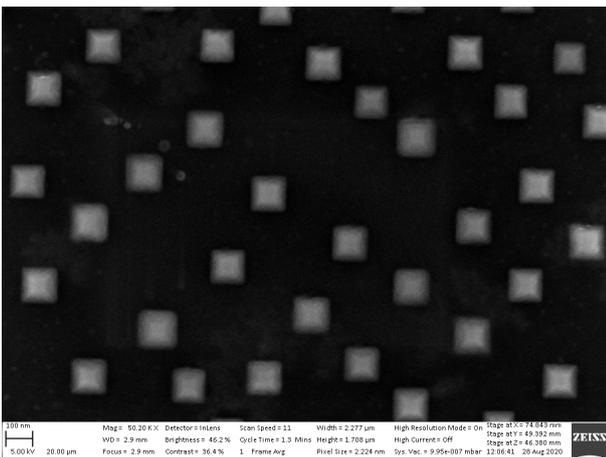

Figure 6: InLens detector at 5kV accelerating voltage and 20um aperture

Using the InLens detector back at a voltage of $V_0 = 5kV$, the SE1 electrons detected with this method deliver a richer image in both contrast and signal to noise ratio. Although still not too sharp, some details on the structure of the crystal islands finally become recognizable, along with some traces of potential contamination to the top left of the sample.
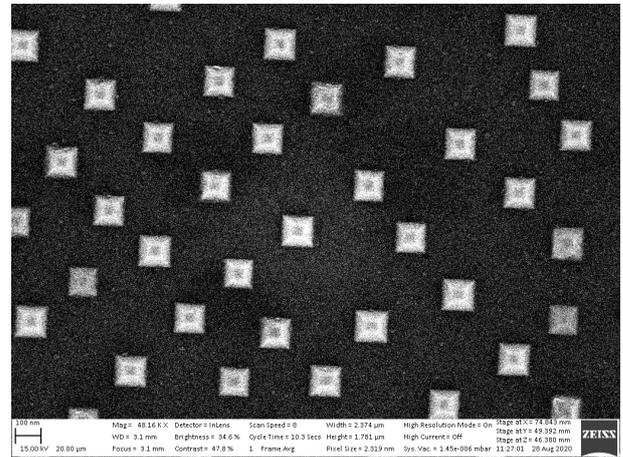

Figure 7: InLens detector at 15kV accelerating voltage and 20um aperture

Moving the imaged area to a less contaminated part and increasing the accelerating voltage back to $V_0 = 15kV$, the image becomes clear and sharp, with a very good contrast and only an increase in the apparent noise as a downside to the higher beam energy used for the imaging of the crystalline structures. The increase in sharpness both here and in Fig.5 can be attributed to the increase in the resolving power of the electron beam at higher acceleration voltages, which causes the DeBroglie wavelength of the electrons to become shorter at $\lambda_e = 17.3pm$ for $V_0 = 5kV$ and $\lambda_e = 9.94pm$ for $V_0 = 15kV$ respectively, therefore increasing their resolving power when imaging smaller structures such as the fine details from the topography of the SiGe crystalline islands. This however, comes at the cost of a reduction in the efficiency of the in-lens detector, as the electrostatic lens which collected the electrons at lower beam energies now accelerates them even further, thus causing the increase in noise.

IV   EDX-Spectroscopy of characteristic X-Rays

For the silicon and germanium within the crystal samples, the following characteristic X-Ray energies can be found in external academic literature [3] and databases [4];

Characteristic X-Ray Energies		
Transition	K-Shell	L-Shell
Silicon	$K_\alpha = 1.74keV$	$L_\alpha = 0.097keV$
	$K_\beta = 1.837keV$	
Germanium	$K_\alpha = 9.886keV$	$L_\alpha = 1.188keV$
	$K_\beta = 10.982keV$	$L_\beta = 1.288keV$

These energies correspond to different, possible transitions of the electrons from higher orbitals falling towards those of lower energy. As can be seen in Fig.3, a K_α transition corresponds to an electron falling to the K-Shell directly from the L-Shell above, whereas a K_β transition occurs when an electron from the higher M-Shell fills in the vacancy inside the K-Shell. Likewise, a L_α transition corresponds to an electron dropping from the M-Shell to the L-Shell directly below, while a L_β transition occurs from the N-Shell. There

can actually be electron transitions of differing energies within the same orbitals due to bonding effects, going by the names of K_{α_1}, K_{α_2} and so on, but within the EDX data, these transition energies and thus characteristic X-Rays are too close together to be resolved individually, so all transitions between the same shells contribute to the same peaks.
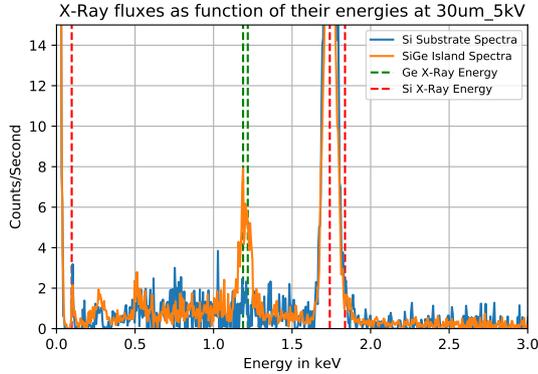

Figure 8: X-Ray emissions 30um aperture and 5kV acceleration voltage

For the graph above, the SiGe sample was focused on at two different points using an electron beam at an accelerating voltage of $V_0 = 5kV$ and with the electronic lens at an aperture of $D = 30um$. The points chosen were on one of the SiGe crystal islands and the Si substrate respectively and correspond with the two spectras shown in the graph. Using these settings, the EDX data shows clear peaks for the silicon $K_\alpha = 1.74keV$ transition both in the spectra for the Si basin at $SiC_{Si} = 45c/s$ as well as the SiGe crystal islands at $SiC_{SiGe} = 29.91c/s$, with the former peak being slightly higher due to what is likely a higher concentration of silicon in the substrate basin due to the abscence of germanium. In addition, a possible peak for the silicon $L_\alpha = 0.097keV$ transition can be seen to the left at around $3c/s$. The peaks for the characteristic X-Ray energies of germanium are only recognizable in the data for the SiGe crystal islands at $GeC_{SiGe} = 8c/s$, indicating a measurably higher concentration of it within the crystals than within the silicon substrate, where any possible peaks GeC_{Si} are indistinguishable from the background noise of the bremsstrahlung.
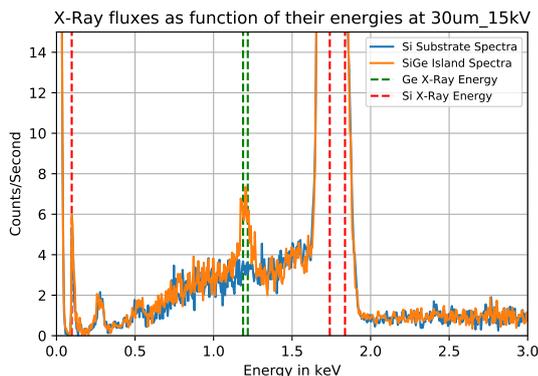

Figure 9: X-Ray emissions at 30um aperture and 15kV acceleration voltage

Increasing the accelerating voltage to $V_0 = 15kV$, the background noise from the bremsstrahlung noticeably increases, as well as the flux readings for the silicon K_α transition peaks which now read about $SiC_{Si} = 430c/s$ and $SiC_{SiGe} = 420.395c/s$ each meanwhile, the readings for the germanium peaks in the SiGe island spectra remain largely unchanged at $GeC_{SiGe} = 8c/s$ and at a value even more indistinguishable from the background noise for the germanium peaks GeC_{Si} within the Si substrate.
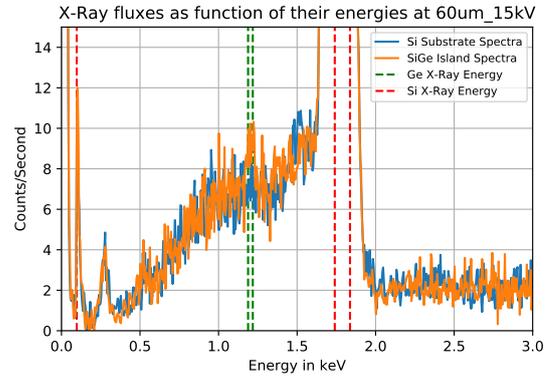

Figure 10: X-Ray emissions at 60um aperture and 15kV electron beam energy

Opening up the aperture D of the electron lens further to $60um$, the resulting increase in the background noise caused by the bremsstrahlung completely drowns out the signal from the germanium peaks, including those belonging to the SiGe crystal islands. This can be explained due to the increased flux of electrons capable of generating bremsstrahlung increasing the flux of X-Rays generated by this process. Contamination of the sample can also contribute to this increased noise which is specially noticeable in the $[0.5; 1.5]keV$ range, with contaminating elements possibly being responsible for unknown peaks such as the one at $0.25keV$ with $5c/s$.

V Elemental Count Maps

The spectra shown in section 4 were measured by focusing the electron beam on given points within the sample, these being either on one of the SiGe crystal islands or the Si substrate. For this section, a progressive scan across the samples topography was made while using the EDX detector to measure the topographic distribution of germanium and silicon within the sample.
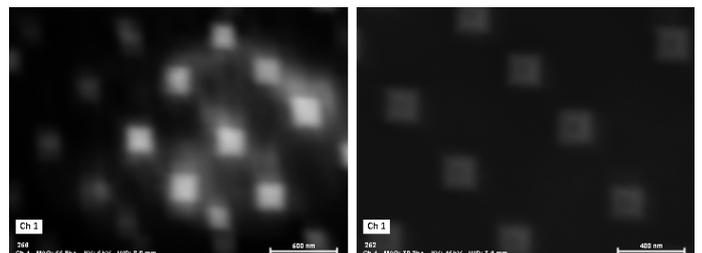

Figure 11: Sample areas for the elemental counts maps, with the area for the map at 5kV left and the area for the map at 15kV right
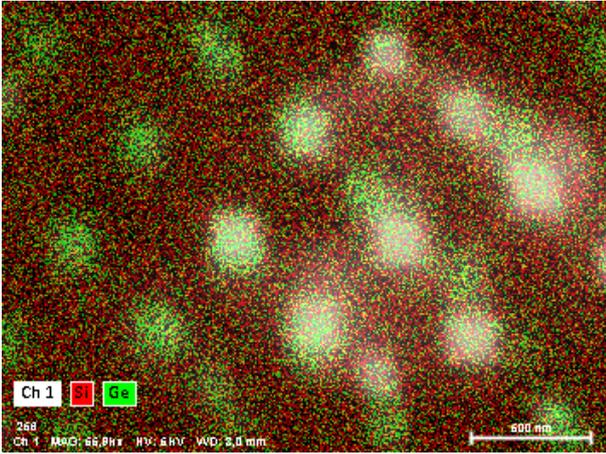
Figure 12: Elemental counts map at 5kV accelerating voltage

At $5kV$ accelerating voltage, the elemental counts map shows a topographic distribution of germanium and silicon consistent with the results from section 4, with the silicon substrate basin showing mainly a silicon composition with only a few traces of germanium, and the SiGe crystal islands holding a much higher concentration of germanium by comparison, to the point that the silicon counts are almost unrecognizable on the islands despite still being present at higher concentrations than germanium.
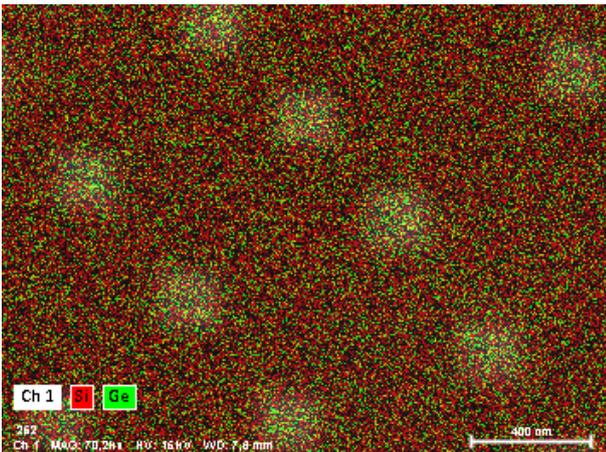

Figure 13: Elemental counts map at 15kV accelerating voltage

A second measurement at $15kV$ accelerating voltage delivers a more consistent mapping with the expected silicon and germanium concentrations on the islands by showing the silicon and germanium counts closer to looking equal than on Fig.12, where the germanium counts seemed to outweight the silicon counts on the SiGe crystals despite the silicon ratio in the islands being known to outweigh the germanium ratio on a 0.6 to 0.4 basis [1]. This discrepancy between Fig.12 and Fig.13 can be attributed to the difference in the c/s readings observed for the silicon peaks in section 4 at the same two accelerating voltages of $5kv$ and $15kv$- for the former, the SiGe silicon counts for the K_α transitions was measured at a peak of $SiC(5kV) = 29.91c/s$, whereas for the later a value one full order of magnitude higher was measured for the counts of the peak at $SiC(15kV) = 420.395c/s$. As the EDX measures and displays elemental counts according to the intensities of the peaks, it must have interpreted the lower silicon counts as a case for a higher germanium ratio, specially at the SiGe islands where germanium counts would be more heavily measured.

VI   Discussion

From the measurements in sections 5 and 6, it can be inferred that the resolving power and accuracy of the imaging detectors as well as the EDX spectra readings for the SEM increase greatly at the higher accelerating voltage $V_0 = 15kV$ of the electron beam, albeit at the cost of both worse signal to noise ratios and damage to the sample. For the imaging of the SiGe islands, the in-lens detector is considerably more efficient at the lower $5kV$ acceleration voltage (Fig.6) and sharper at $15kV$ (Fig.7) than the SE2 detector (Figs. 4/5)- albeit this could also depend at some degree on other factors outside the detection efficiency of either device, as the sample quality was sufficiently compromised by the lack of time for proper inspection and preparation.

This was specially noticeable during the measurements using the EDX spectrometer, where the noise readings at the higher accelerating voltage of $15kV$ (Fig.9) and aperture of $D = 60mm$ (Fig.10) were high enough to drown out any peaks for the germanium emissions, indicating a potentially contaminated sample as unknown peaks from materials other than silicon and germanium could also be observed, thus contributing to the overall noise alongside the characteristic Bremsstrahlung background signal, and forcing the measurements to be carried out at $5kV$ accelerating voltage and $30um$ aperture (Fig.8) for an acceptable signal to noise ratio.

For a more accurate assesment on the detection efficiency of the SEM at its different settings and utilizing various detection methods, a cleaner, more careful preparation of the sample would thus potentially be of benefit in future inquiries.

VII   References

[1] Dr. W.Van den Broek, A.Parvizi, H.Kirmse, C.T.Koch: *Spatially-Resolved Elemental Analysis in the Scanning Electron Microscope*, Humboldt University Physics Institute, 2020

[2] Dr. Bob Hafner: *Energy Dispersive Spectroscopy on the SEM: A Primer*, University of Minnesota, 2019

[3] Bruker: *Periodic Table of Elements and X-ray Energies* , www.bruker.com/hhxrf

[4] NIST: *X-Ray Transition Energies Database*, https://physics.nist.gov/PhysRefData/XrayTrans/Html/searc

VIII   Measurements and Computations

ScanningElectronMicroscope

October 18, 2020

1 Imaging of Si-Ge Crystal Sctructures using a Scanning Electron Microscope (SEM)

Santiago.R MN: 598454

```
[75]: import numpy as np
      import scipy.constants as cs
      import matplotlib.pyplot as plt
      import pandas
      from PIL import Image
      data_path="/home/santi/Documents/Arbeits-Dokumente/Experimental Data/"
```

2 De-Broglie Wavelength λ_e for Electrons with different Acceleration Voltages V_0

The DeBroglie wavelength capable of describing the wave nature properties of mass-carrying particles is given by $\lambda_e = \frac{hc}{\sqrt{eV_0(2m_0c^2+eV_0)}}$ This relation can be evaluated repeatedly according to input voltage or electron wavelength by defining the following functions;

Functions

```
[76]: #Constants
      h = cs.Planck
      m_0 = cs.electron_mass
      c = cs.speed_of_light
      e = cs.elementary_charge
      #Function returning the Electron wavelenght in pm at a given accelerating␣
       ↪Voltage in kV
      def electron_wavelength(V_0):
          V_0 = V_0*1000 #Conversion to volt
          debroglie_wavelength = h*c/(np.sqrt(e*V_0*(2*m_0*c**2+e*V_0)))
          debroglie_wavelength = debroglie_wavelength*10**12 #Conversion to picometers
          return debroglie_wavelength
```

```
[77]: #Electron wavelength curve as a function of the accelerating Voltage between 1kV␣
       ↪and 100kV
```

1

```
V_e = np.linspace(1,20,10000)
plt.plot(V_e,electron_wavelength(V_e))
plt.vlines(5, np.zeros(1),40, label='5kV', color='lightblue',␣
 ↪linestyle='dashed')        #Plot characteristic X-Ray energies for Ge
plt.vlines(15, np.zeros(1),40, label='15kV', color='darkblue',␣
 ↪linestyle='dashed')         #Plot characteristic X-Ray energies for Si
plt.xlabel('Accelerating voltage in kV')
plt.ylabel('DeBroglie wavelength in pm')
plt.legend()
startx, endx = 0, 20
starty, endy = 0, 40
plt.axis([startx, endx, starty, endy])
plt.show()
print('The wavelength becomes shorter for increased accelerating voltages, but␣
 ↪converges towards zero at higher values with higher voltages reducing the␣
 ↪wavelength less and less')
#Compute the electron wavelength for the 5kV and 15kV beam energies
V_sem = np.array([5,15])
print('The DeBroglie wavelength of the electrons accelerated in the SEM at␣
 ↪energies of', V_sem , 'keV is' ,electron_wavelength(V_sem), 'pm respectively')
```
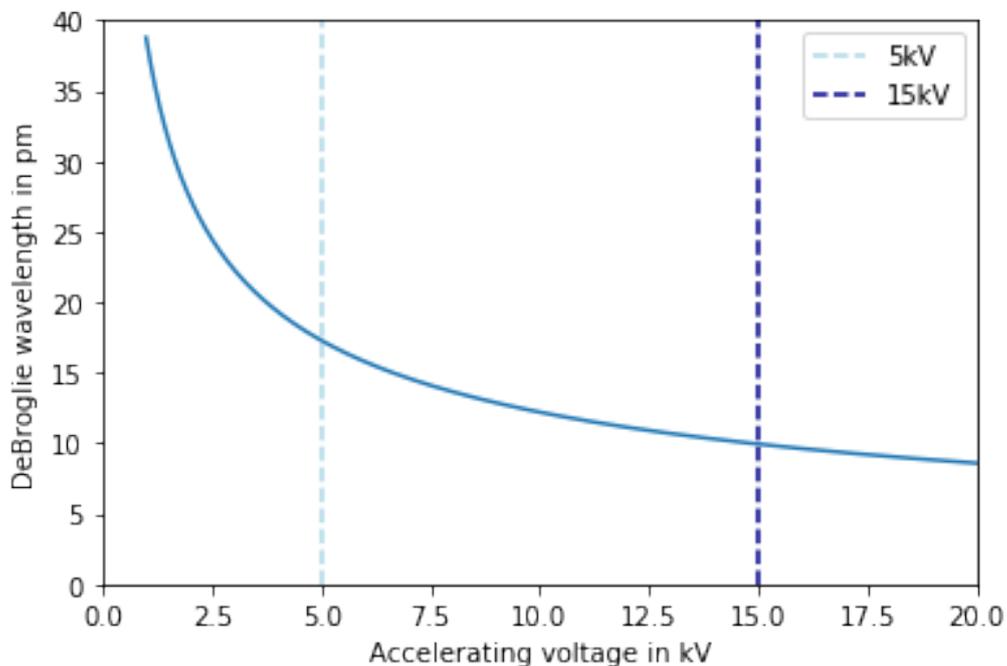

The wavelength becomes shorter for increased accelerating voltages, but
converges towards zero at higher values with higher voltages reducing the
wavelength less and less

The DeBroglie wavelength of the electrons accelerated in the SEM at energies of
[5 15] keV is [17.30201   9.94103884] pm respectively

Accelerating Voltage Function

The energy of a mass-carrying particle at a given DeBroglie wavelength thus becomes: $E = \sqrt{(\frac{hc}{\lambda})^2 + m_0^2 c^4}$

```
[78]: #Function returning the neccessary accelerating Voltage for a given Electron␣
      ↪Wavelength
      def accelerating_voltage(debroglie_wavelength):
          d = debroglie_wavelength
          V_0 = (np.sqrt((h*c/d)**2+m_0**2*c**4)-m_0*c**2)/e
          return V_0
```

```
[79]: electron_wavelength(1000) #Test for 1kV
```

```
[79]: 0.8719186929043307
```

```
[80]: accelerating_voltage(3.8764034152582323e-11) #Test for 38.7pm wavelength
```

```
[80]: 1000.0000000000866
```

For the experiment, accelerating voltages of 5kV and 15kV were used, which corresponds to

```
[81]: sem_voltages = np.array([15000,5000])
      electron_wavelength(sem_voltages)
```

```
[81]: array([0.0799765 , 0.22594932])
```

Photon energies E_{ph} at similar wavelengths λ

```
[82]: #Function for the energy E of a photon of wavelength lambda in pm given in keV
      def photon_energy(wavelength_pm):
          w = wavelength_pm*10**(-12)
          E = h*c/w
          E = E/(e*1000) #conversion to keV
          return E
```

```
[83]: photon_energy(electron_wavelength(V_sem))
```

```
[83]: array([ 71.65884105, 124.71955941])
```

Uncertainties

Assuming only an uncertainty for the accelerating voltage V_0, the gaußian error proprogation becomes $u_{\lambda_e} = u_{V_0} \cdot \frac{hce(m_0 c^2 + eV_0)}{\sqrt{eV_0(2m_0 c^2 + eV_0)}}$ Which may then be automatically computed alongside the electron wavelength with

3

```
[84]: def electron_wavelength_err(V_0,u_V):
          debroglie_wavelength = h*c/(np.sqrt(e*V_0*(2*m_0*c**2+e*V_0)))
          err = u_V*h*c*e*(m_0*c**2+e*V_0)/(np.sqrt(e*V_0*(2*m_0*c**2+e*V_0)))
          return debroglie_wavelength, err
```

```
[85]: electron_wavelength_err(20000,100) #Test for 20kV and 100V uncertainty
```

```
[85]: (8.58851184477148e-12, 1.170664284336823e-41)
```

This uncertainty is comparatively low when compared to the computed value for the electrons wavelength

3   Scanning Electron Microscope Data Processing

Image Evaluation

The data from the SEM is saved as TIFF files. These files can be read using PIL as follows;
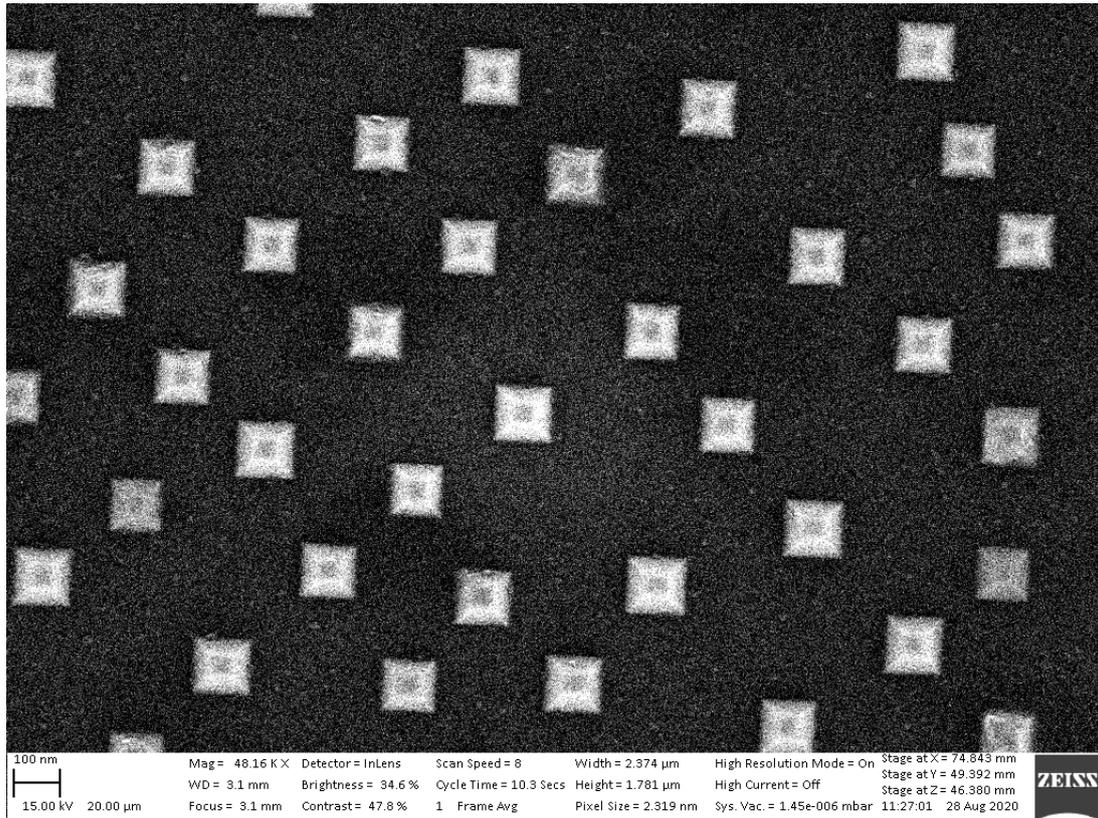
```
[86]: #Open TIFF with PIL.Image
      im = Image.open('SEM/15kV_InLens_3mm.tif')
      im.show()
```

```
[87]: #Convert TIFF to Numpy Array
      imarray = np.array(im)
      print(imarray)
```

```
[[125  24   0 ...  12   0  49]
 [  8  18  31 ...  54  24   0]
 [ 62   8  97 ...  17   0  22]
 ...
 [ 46 255 255 ... 255 255 247]
 [  0 255 255 ... 255 255 121]
 [ 59  26   0 ... 212 195 196]]
```

```
[88]: #Save Numpy Array as TIFF again
      Image.fromarray(imarray)
```

```
[88]:
```

4 Characteristic X-Ray Spectroscopy

Functions and Constants

The characteristic X-Ray energies for Germanium (Ge) and Silicon (Si) are in KeV

```
[89]:  ge_energies = np.array([9.886,10.982,1.188,1.218])    #in order from left to
       →right; K-Alpha, K-Beta, L-Alpha, L-Beta transitions
       si_energies = np.array([1.740,1.837,1.837-1.74])              #in order from
       →left to right; K-Alpha, K-Beta transitions
```

From $E = \frac{hc}{\lambda} \Leftrightarrow \lambda = \frac{hc}{E}$ it then follows for the X-Ray wavelengths that

```
[90]:  def photon_wavelength(E):
           E_V = E*1000*e              #for E in keV
           lmbd = h*c/E_V
           return lmbd
```

Thus, for the characteristic Germanium (Ge) X-Ray wavelengths it holds true that

```
[91]: Ge_Wavelengths = photon_wavelength(ge_energies)*10**9 #in mm
      print('The characteristic wavelengths for Germanium X-Ray emissions are',␣
       ↪Ge_Wavelengths, 'nm')
```

The characteristic wavelengths for Germanium X-Ray emissions are [0.12541392
0.11289765 1.04363803 1.01793266] nm

and for Silicon (Si)

```
[92]: Si_Wavelengths = photon_wavelength(si_energies)*10**9 #in mm
      print('The characteristic wavelengths for Silicon X-Ray emissions are',␣
       ↪Si_Wavelengths, 'nm')
```

The characteristic wavelengths for Silicon X-Ray emissions are [0.71255286
0.67492759 12.78187613] nm

Spectra Evaluations

The data from the EDX detector measuring the X-Ray spectra is saved in xlsx files.
These files can be read using Pandas as follows;

```
[93]: lower_energy_si_ge = pandas.read_excel('SEM/30um_5kV_SiGe.xlsx')          ␣
       ↪#Spectra of a SiGe crystal island at 5kV beam energy and 30um aperture
      lower_energy_si = pandas.read_excel('SEM/30um_5kV_Si.xlsx')               ␣
       ↪#Spectra of the Si basion at 5kV beam energy and 30um aperture
      higher_energy_si_ge = pandas.read_excel('SEM/30um_15kV_SiGe.xlsx')        ␣
       ↪#Spectra of a SiGe crystal island at 15kV beam energy and 30um aperture
      higher_energy_si = pandas.read_excel('SEM/30um_15kV_Si.xlsx')             ␣
       ↪#Spectra of the Si basin at 15kV beam energy and 30um aperture
      higher_energy_aperture_si_ge = pandas.read_excel('SEM/60um_15kV_SiGe_1.xlsx') ␣
       ↪#Spectra of the SiGe crystal island at 15kV beam energy and 60um aperture
      higher_energy_aperture_si = pandas.read_excel('SEM/60um_15kV_Si.xlsx')    ␣
       ↪#Spectra of the Si basin at 15kV beam energy and 60um aperture
      #---------------------------------------------------------------
      sample_si = np.array([1000,1000])            #Sample Counts for the Si X-Ray␣
       ↪energies
      sample_ge = np.array([1000,1000,1000,1000])    #Sample Counts for the Ge X-Ray␣
       ↪energies
```

Now, in order to read into the spectras, the xlsx files store the data starting
from the 26th row, with the 1st column giving the measurement number, the 2nd the
measured Energy, the 3rd the measured counts, and the 4th the counts/second

```
[94]: #Plot for the Spectra of a SiGe crystal island at 5kV beam energy and 30um␣
       ↪aperture
      low_si_ge_energy_readings = lower_energy_si_ge.values[25:,1]              ␣
       ↪#Write Energy readings to a Numpy Array
      low_si_ge_count_readings = lower_energy_si_ge.values[25:,3]              ␣
       ↪#Write Count/Seconds readings to a Numpy Array
```

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```
plt.plot(low_si_ge_energy_readings,low_si_ge_count_readings)           ␣
 ↪#Plot the data
plt.vlines(ge_energies, np.zeros(4),sample_ge, label='Ge', color='green',␣
 ↪linestyle='dashed')        #Plot characteristic X-Ray energies for Ge
plt.vlines(si_energies, np.zeros(2),sample_si, label='Si', color='red',␣
 ↪linestyle='dashed')          #Plot characteristic X-Ray energies for Si
plt.xlabel('Energy in keV')
plt.ylabel('Counts/Second')
plt.legend()
plt.grid(True)
startx, endx = 0, 3
starty, endy = 0, low_si_ge_count_readings[444]
plt.axis([startx, endx, starty, endy])
plt.savefig('Plots/30um_5kV_SiGe.pdf')
plt.show()
```
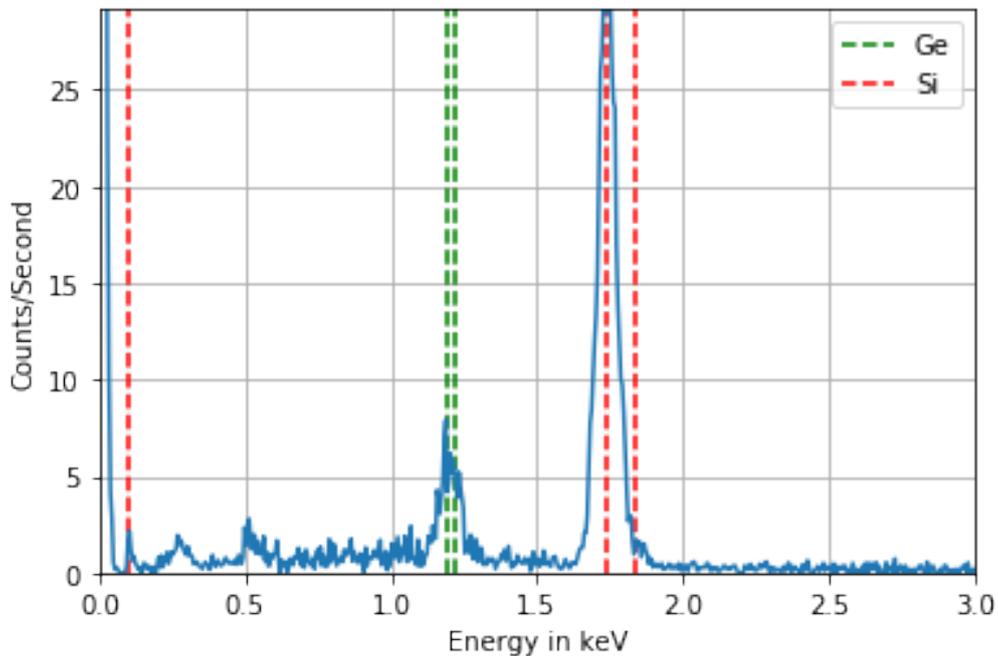

The same evaluation can then be repeated efficiently for the other measurements by
defining a function

```
[95]: def xspectra_evaluation(EDX_data, x_boundaries, y_boundaries, file_name):
          energy_readings = EDX_data.values[25:,1]                              ␣
       ↪    #Write Energy readings to a Numpy Array
          cps_readings = EDX_data.values[25:,3]                                 ␣
       ↪    #Write Count/Seconds readings to a Numpy Array
```

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```
    plt.plot(energy_readings,cps_readings)                              ␣
↪   #Plot the data
    plt.vlines(ge_energies, np.zeros(4),sample_ge, label='Ge', color='green',␣
↪linestyle='dashed')        #Plot characteristic X-Ray energies for Ge
    plt.vlines(si_energies, np.zeros(2),sample_si, label='Si', color='red',␣
↪linestyle='dashed')        #Plot characteristic X-Ray energies for Si
    plt.xlabel('Energy in keV')
    plt.ylabel('Counts/Second')
    plt.legend()
    plt.grid(True)
    startx, endx = x_boundaries
    starty, endy = y_boundaries
    plt.axis([startx, endx, starty, endy])
    plt.savefig('Plots/' + file_name + '.pdf')
    plt.show
```
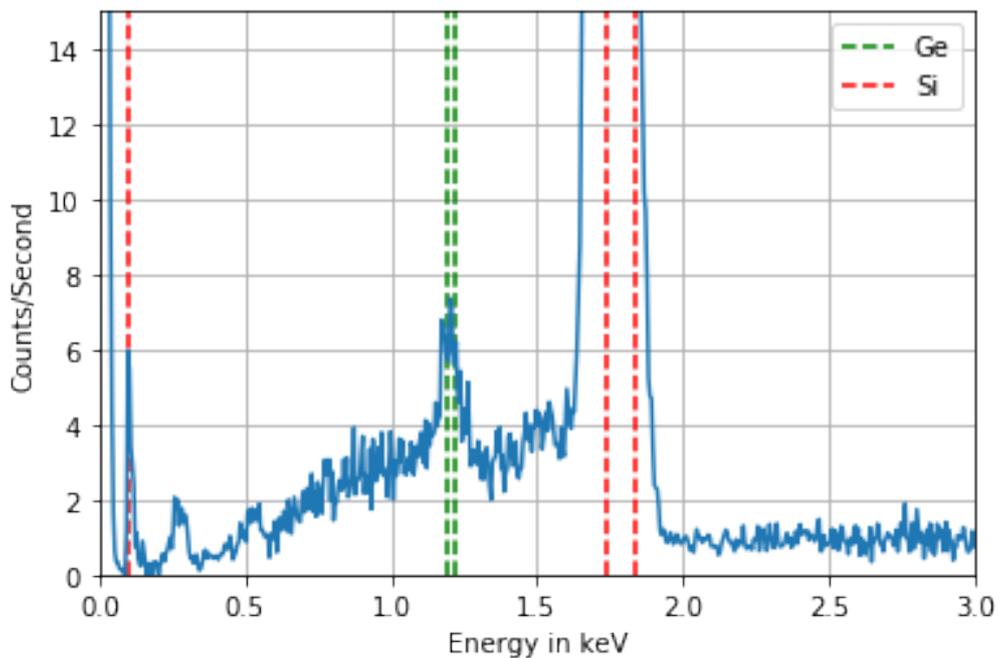
```
[96]: #Plot for the Spectra of the Si basin at 5kV beam energy and 30um aperture from␣
↪9-12 keV
x_boundary_5kV = np.array([0,3])
y_boundary_5kV = np.array([0,60])
xspectra_evaluation(lower_energy_si, x_boundary_5kV, y_boundary_5kV,␣
↪'30um_5kV_Si')
```
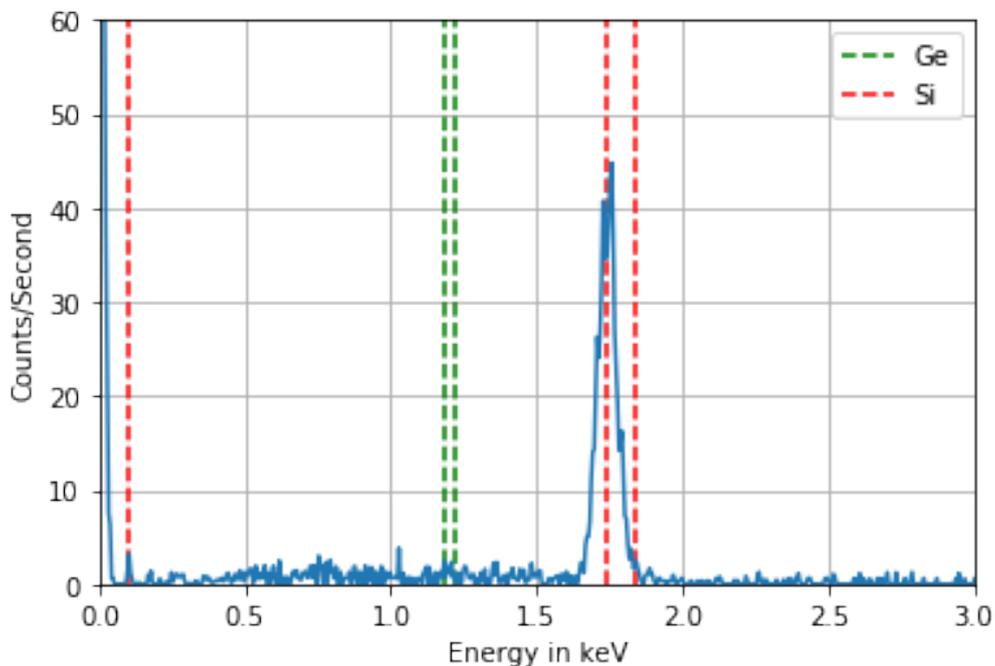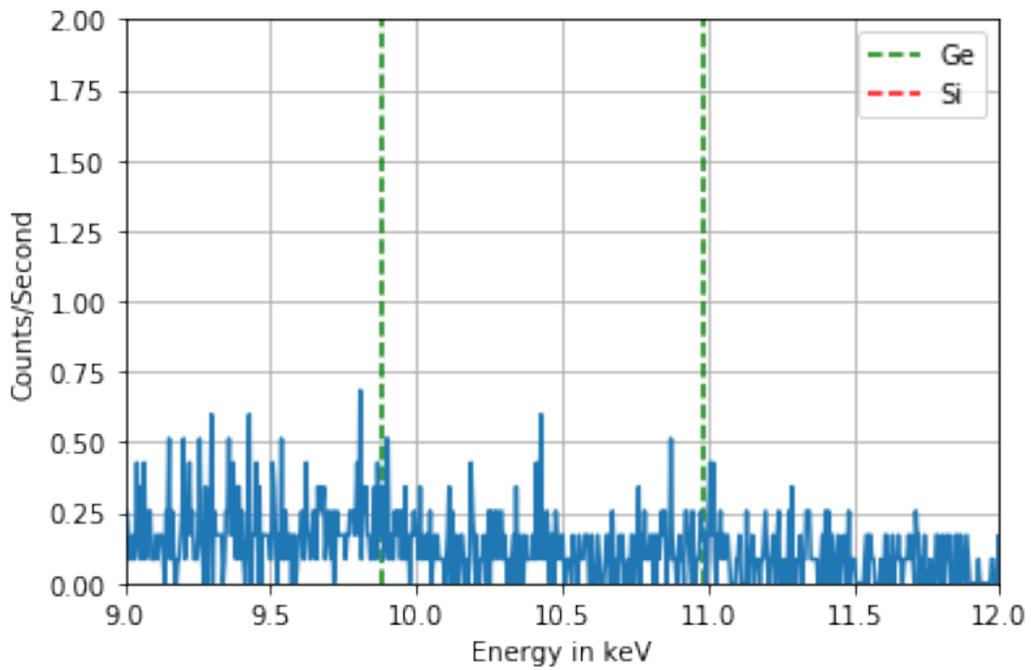
```
[97]: #Plot for the Spectra of a SiGe crystal island at 15kV beam energy and 30um␣
      ↪aperture from 0-3 keV
      x_boundary_15kV_1 = np.array([0,3])
      y_boundary_15kV_1 = np.array([0,15])
      xspectra_evaluation(higher_energy_si_ge, x_boundary_15kV_1, y_boundary_15kV_1,␣
      ↪'30um_15kV_SiGe')
```
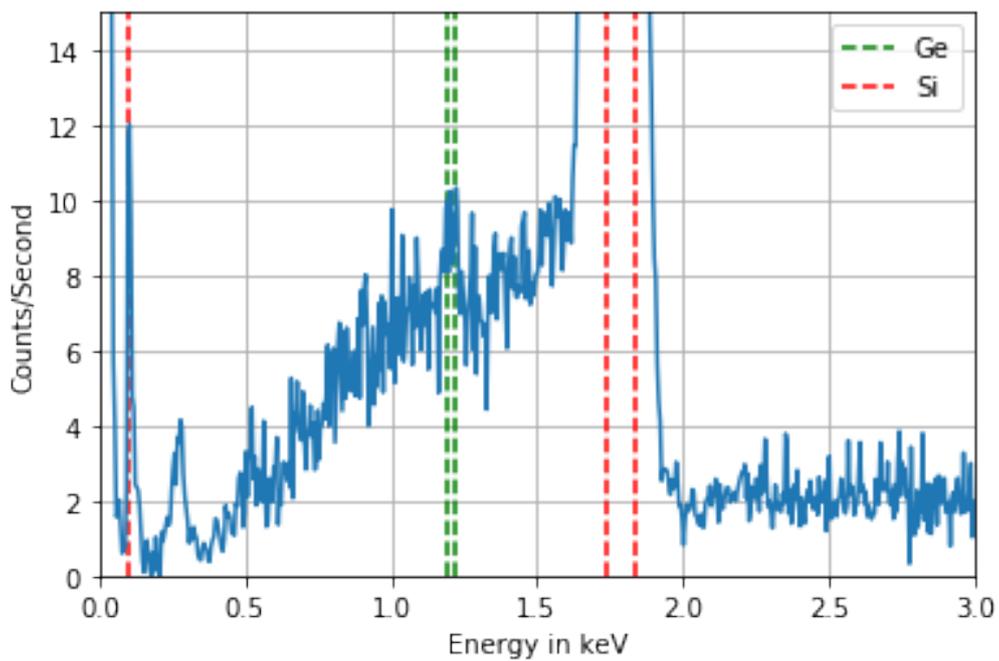


```
[98]: #Plot for the Spectra of a SiGe crystal island at 15kV beam energy and 30um␣
      ↪aperture from 9-12 keV
      x_boundary_15kV_2 = np.array([9,12])
      y_boundary_15kV_2 = np.array([0,2])
      xspectra_evaluation(higher_energy_si_ge, x_boundary_15kV_2, y_boundary_15kV_2,␣
      ↪'30um_15kV_SiGe2')
```
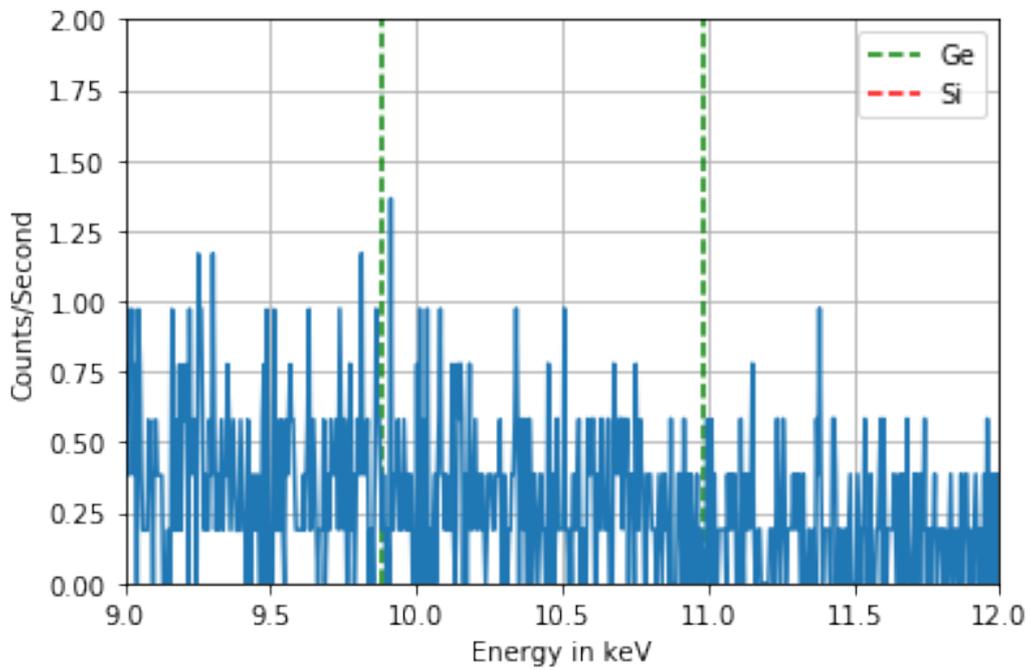
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```
[99]: #Plot for the Spectra of the Si basin at 15kV beam energy and 30um aperture
       xspectra_evaluation(higher_energy_si, x_boundary_15kV_1, y_boundary_15kV_1,␣
        ↪'30um_15kV_Si')
```


10
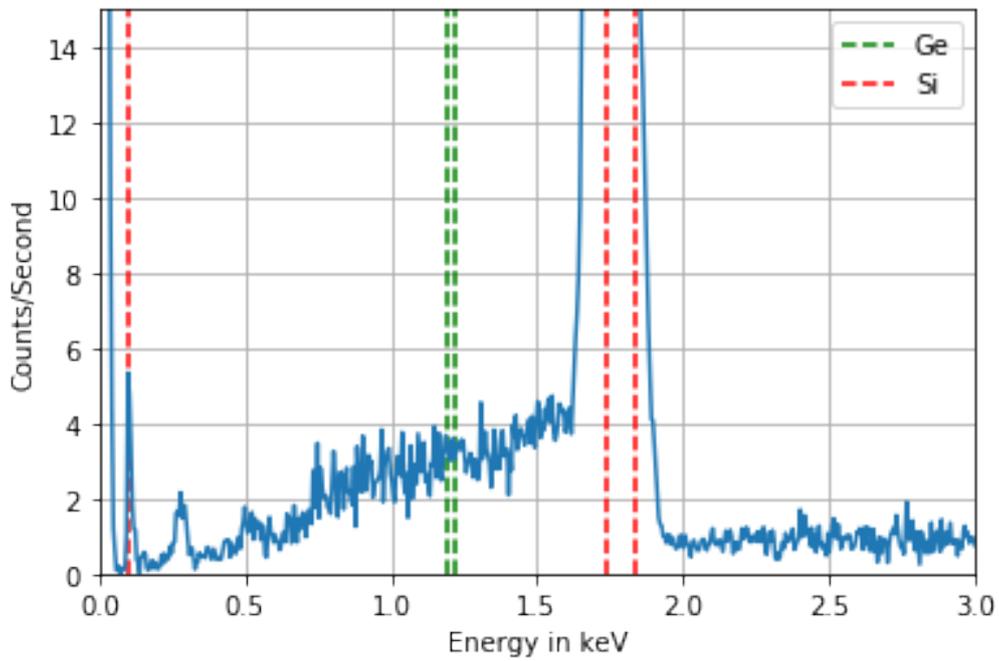
```
[100]: #Plot for the Spectra of the SiGe crystal island at 15kV beam energy and 60um␣
       ↪aperture
       xspectra_evaluation(higher_energy_aperture_si_ge, x_boundary_15kV_1,␣
       ↪y_boundary_15kV_1, '60um_15kV_SiGe')
```



```
[101]: #Plot for the Spectra of the SiGe crystal island at 15kV beam energy and 60um␣
       ↪aperture
       xspectra_evaluation(higher_energy_aperture_si_ge, x_boundary_15kV_2,␣
       ↪y_boundary_15kV_2, '60um_15kV_SiGe2')
```

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```
[102]:  #Plot for the Spectra of the Si basin at 15kV beam energy and 60um aperture
        xspectra_evaluation(higher_energy_aperture_si, x_boundary_15kV_1,␣
        ↪y_boundary_15kV_1, '60um_15kV_Si')
```


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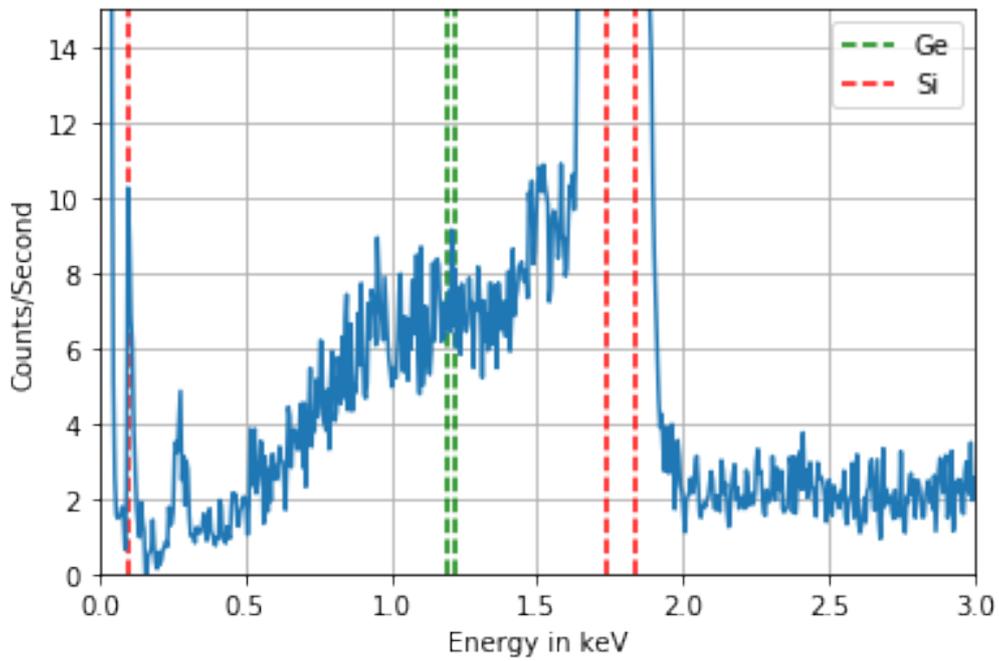
```
[140]:  #Plot for all the Spectra of the SiGe crystal island between 8 and 12 keV
        energy_readings = lower_energy_si_ge.values[25:,1]                            ␣
        →         #Write Energy readings to a Numpy Array
        cps_readings = lower_energy_si_ge.values[25:,3]                               ␣
        →         #Write Count/Seconds readings to a Numpy Array
        plt.plot(energy_readings,cps_readings, color='orange')                        ␣
        →                       #Plot the data
        energy_readings = higher_energy_si_ge.values[25:,1]                           ␣
        →         #Write Energy readings to a Numpy Array
        cps_readings = higher_energy_si_ge.values[25:,3]                              ␣
        →         #Write Count/Seconds readings to a Numpy Array
        plt.plot(energy_readings,cps_readings, color='blue')                          ␣
        →                       #Plot the data
        energy_readings = higher_energy_aperture_si_ge.values[25:,1]                  ␣
        →         #Write Energy readings to a Numpy Array
        cps_readings = higher_energy_aperture_si_ge.values[25:,3]                     ␣
        →         #Write Count/Seconds readings to a Numpy Array
        plt.plot(energy_readings,cps_readings, color='brown')                         ␣
        →                       #Plot the data
        plt.vlines(ge_energies, np.zeros(4),sample_ge, label='Ge', color='green',␣
        →linestyle='dashed')        #Plot characteristic X-Ray energies for Ge
        plt.vlines(si_energies, np.zeros(2),sample_si, label='Si', color='red',␣
        →linestyle='dashed')          #Plot characteristic X-Ray energies for Si
        plt.xlabel('Energy in keV')
        plt.ylabel('Counts/Second')
        plt.legend()
        plt.grid(True)
        startx, endx = x_boundary_15kV_2
        starty, endy = y_boundary_15kV_2
        plt.axis([startx, endx, starty, endy])
        file_name = '15kV_SiGe2'
        plt.savefig('Plots/' + file_name + '.pdf')
        plt.show
```

```
[140]: <function matplotlib.pyplot.show(*args, **kw)>
```

13
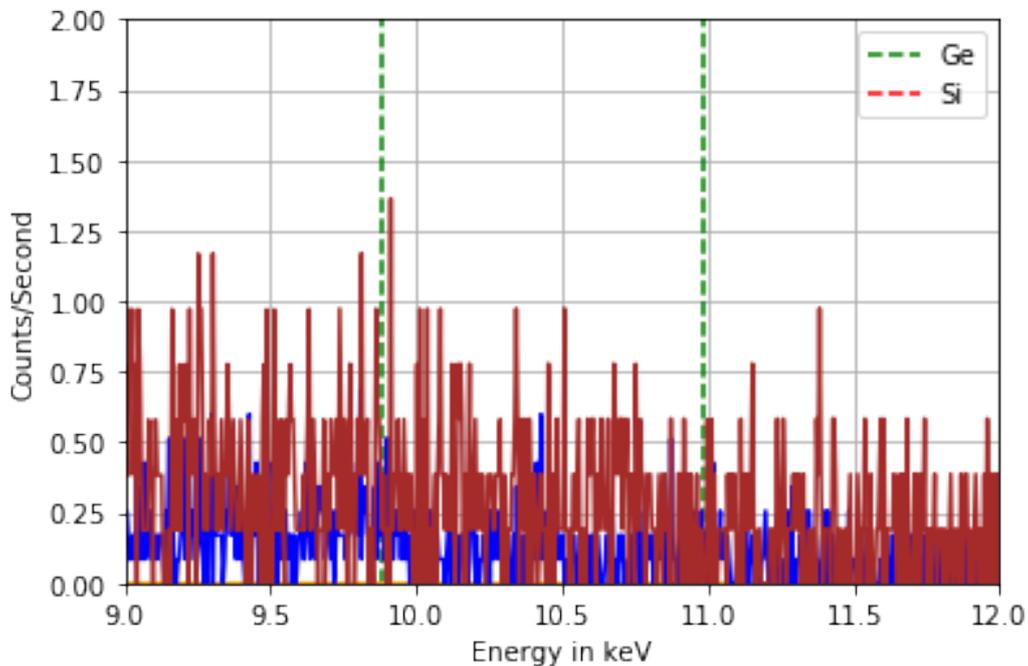
Multiple Spectra Plots

```python
def multispectra_evaluation(EDX_datasets, x_boundaries, y_boundaries, file_name):
    i = len(EDX_datasets)
    data_names = ['Si Substrate Spectra', 'SiGe Island Spectra']
    for i in range(0,i,1):
        EDX_data = EDX_datasets[i]
        data_name = data_names[i]
        energy_readings = EDX_data.values[25:,1]          #Write Energy readings to a Numpy Array
        cps_readings = EDX_data.values[25:,3]             #Write Count/Seconds readings to a Numpy Array
        plt.plot(energy_readings,cps_readings, label = data_name)          #Plot the data
    plt.vlines(ge_energies, np.zeros(4),sample_ge, label='Ge X-Ray Energy',color='green', linestyle='dashed')       #Plot characteristic X-Ray energies for Ge
    plt.vlines(si_energies, np.zeros(2),sample_si, label='Si X-Ray Energy',color='red', linestyle='dashed')       #Plot characteristic X-Ray energies for Si
    plt.xlabel('Energy in keV')
    plt.ylabel('Counts/Second')
    plt.legend(loc = 'upper right', prop={'size': 8})
    plt.grid(True)
```

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```
        plt.title('X-Ray fluxes as function of their energies at ' + file_name)
        startx, endx = x_boundaries
        starty, endy = y_boundaries
        plt.axis([startx, endx, starty, endy])
        plt.savefig('Plots/' + file_name + '.pdf')
        plt.show
```

[131]:
```
EDX_datasets_5kV = [lower_energy_si, lower_energy_si_ge]
x_boundary_5kV = np.array([0,3])
y_boundary_5kV = np.array([0,15])
multispectra_evaluation(EDX_datasets_5kV, x_boundary_5kV, y_boundary_5kV,␣
 ↪'30um_5kV')
```
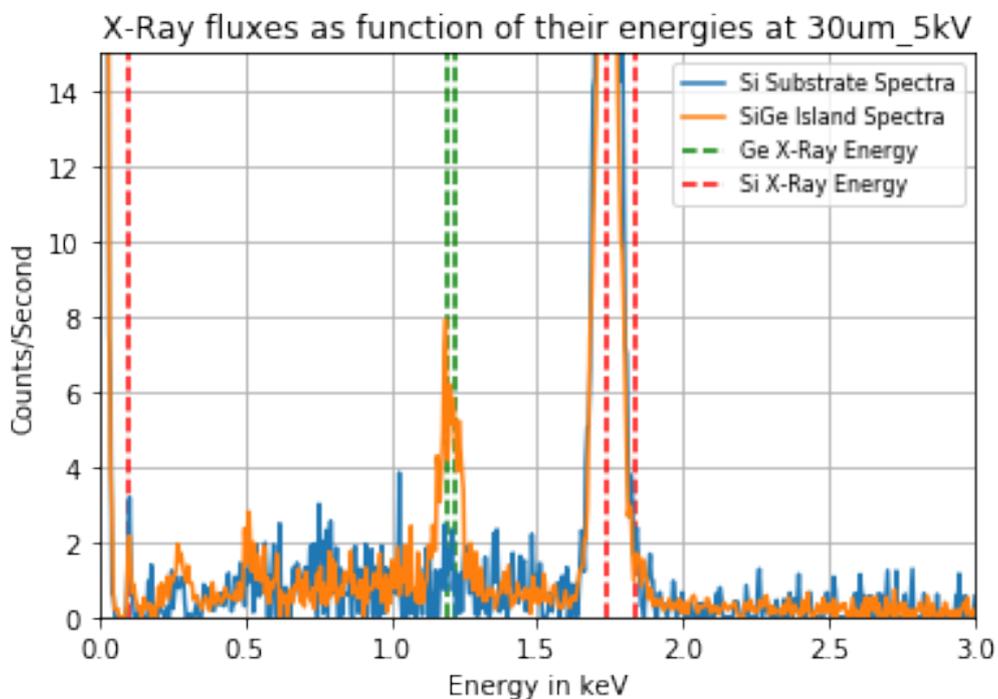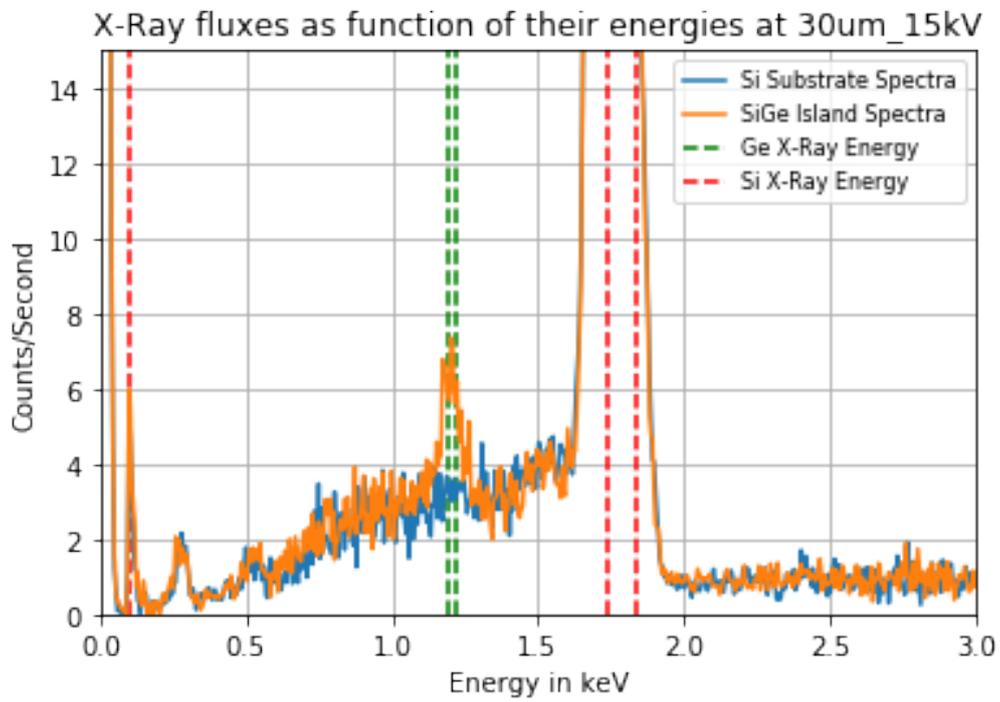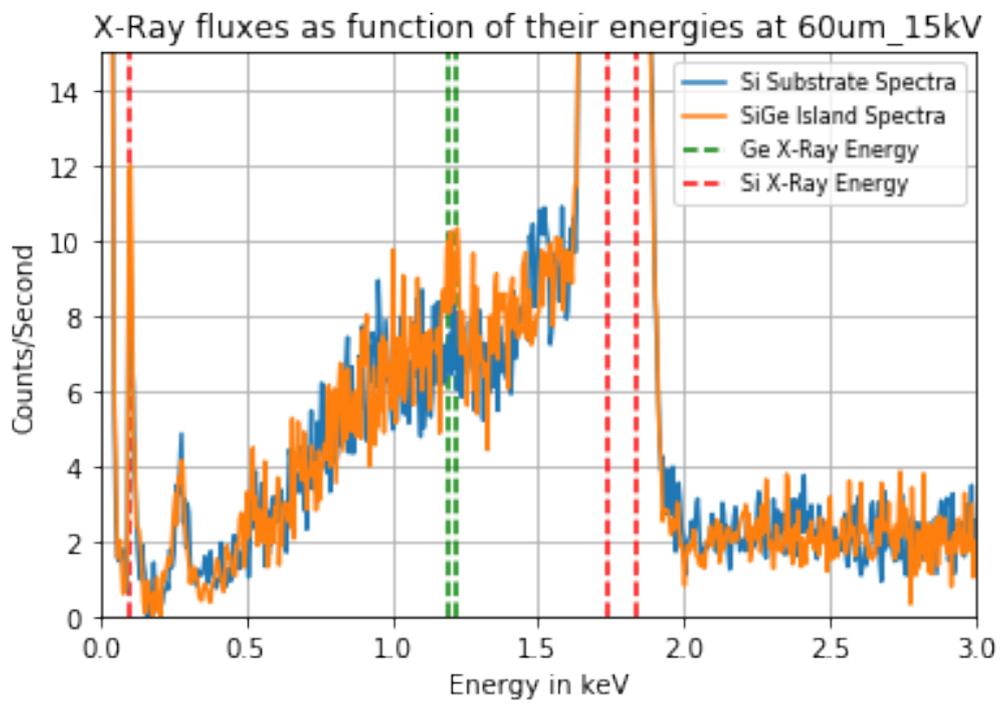

[130]:
```
EDX_datasets_15kV = [higher_energy_si, higher_energy_si_ge]
x_boundary_15kV = np.array([0,3])
y_boundary_15kV = np.array([0,15])
multispectra_evaluation(EDX_datasets_15kV, x_boundary_15kV, y_boundary_15kV,␣
 ↪'30um_15kV')
```

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X-Ray fluxes as function of their energies at 30um_15kV


```
[121]: EDX_datasets_15kV_60um = [higher_energy_aperture_si,␣
       ↪higher_energy_aperture_si_ge]
       multispectra_evaluation(EDX_datasets_15kV_60um, x_boundary_15kV,␣
       ↪y_boundary_15kV, '60um_15kV')
```

X-Ray fluxes as function of their energies at 60um_15kV

[ ]: