XPCS3

November 2, 2015

1 XPCS Pipeline

“This notebook corresponds to version {{ version }} of the pipeline tool: https://github.com/NSLS-II/pipelines”

1.1 NSLS2 data retrieval imports

In [1]:
```
from databroker import DataBroker as db, get_images, get_table, get_events
from filestore.api import register_handler, deregister_handler
from filestore.retrieve import _h_registry, _HANDLER_CACHE
```

In [2]:
```
#hdr = db[{{ uid }}]
```

In [3]:
```
import numpy as np
import matplotlib as mpl
import matplotlib.pyplot as plt
from matplotlib.colors import LogNorm
```

1.1.1 Lazy Eiger Handler (later will goto databroker)

In [4]:
```
import h5py
from filestore.retrieve import HandlerBase
from eiger_io.pims_reader import EigerImages

EIGER_MD_DICT = {
    'y_pixel_size': 'entry/instrument/detector/y_pixel_size',
    'x_pixel_size': 'entry/instrument/detector/x_pixel_size',
    'detector_distance': 'entry/instrument/detector/detector_distance',
    'incident_wavelength': 'entry/instrument/beam/incident_wavelength',
    'frame_time': 'entry/instrument/detector/frame_time',
    'beam_center_x': 'entry/instrument/detector/beam_center_x',
    'beam_center_y': 'entry/instrument/detector/beam_center_y',
    'count_time': 'entry/instrument/detector/count_time',
    'pixel_mask': 'entry/instrument/detector/detectorSpecific/pixel_mask',
}

class FixedEigerImages(EigerImages):
    def __init__(self, path, metadata):
        super().__init__(path)
        self._metadata = metadata

    @property
    def md(self):
        return self._metadata
```

```python
    @property
    def dtype(self):
        return self.pixel_type

    @property
    def shape(self):
        return self.frame_shape

class LazyEigerHandler(HandlerBase):
    specs = {'AD_EIGER'} | HandlerBase.specs
    def __init__(self, fpath, frame_per_point, mapping=None):
        # create pims handler
        self.vals_dict = EIGER_MD_DICT.copy()
        if mapping is not None:
            self.vals_dict.update(mapping)
        self._base_path = fpath
        self.fpp = frame_per_point

    def __call__(self, seq_id):
        import h5py
        master_path = '{}_{}_master.h5'.format(self._base_path, seq_id)
        md = {}
        print('hdf5 path = %s' % master_path)
        with h5py.File(master_path, 'r') as f:
            md = {k: f[v].value for k, v in self.vals_dict.items()}
        # the pixel mask from the eiger contains:
        # 1  -- gap
        # 2  -- dead
        # 4  -- under-responsive
        # 8  -- over-responsive
        # 16 -- noisy
        pixel_mask = md['pixel_mask']
        pixel_mask[pixel_mask>0] = 1
        pixel_mask[pixel_mask==0] = 2
        pixel_mask[pixel_mask==1] = 0
        pixel_mask[pixel_mask==2] = 1
        md['framerate'] = 1./md['frame_time']
        # TODO Return a multi-dimensional PIMS seq
        return FixedEigerImages(master_path, md)

deregister_handler('AD_EIGER')
_HANDLER_CACHE.clear()
register_handler('AD_EIGER', LazyEigerHandler)
```

In [5]:
```python
#%matplotlib notebook
%matplotlib inline
```

1.1.2 Get the events from the uid

In [6]:
```python
def print_attrs(name, obj):
    print(name)
    for key, val in obj.attrs.items():
        print("    %s: %s" % (key, val))
```

```
#f = h5py.File('/XF11ID/data/2015/10/16/bcdd8b95-6adc-476b-9c65_25_master.h5','r')
#f.visititems(print_attrs)
```

```
In [7]: uid = '8a3f3e04'
```

```
In [8]: hdr = db[uid]
```

```
In [9]: ev, = get_events(hdr, ['eiger_4M_cam_img_image_lightfield'], fill = True)
```

```
hdf5 path = /XF11ID/data/2015/10/30/ad0ec08c-201e-4723-a8a6_9093_master.h5
```

```
In [10]: imgs = ev['data']['eiger_4M_cam_img_image_lightfield']
         print (imgs)
         Nimg=len(imgs)
```

```
<Frames>
Length: 2500 frames
Frame Shape: 2167 x 2070
Pixel Datatype: uint16
```

```
In [11]: imgs.md
```

```
Out[11]: {'beam_center_x': 840.0,
          'beam_center_y': 336.0,
          'count_time': 0.0049999999,
          'detector_distance': 4.8400002,
          'frame_time': 0.00501,
          'framerate': 199.60079982206346,
          'incident_wavelength': 1.3794414,
          'pixel_mask': array([[1, 1, 1, ..., 1, 1, 0],
                 [1, 1, 1, ..., 1, 1, 1],
                 [1, 1, 1, ..., 1, 1, 1],
                 ...,
                 [1, 1, 1, ..., 1, 1, 1],
                 [1, 1, 1, ..., 1, 1, 1],
                 [1, 1, 1, ..., 1, 1, 1]], dtype=uint32),
          'x_pixel_size': 7.5000004e-05,
          'y_pixel_size': 7.5000004e-05}
```

2 get masks

```
In [12]: class RemoveHotSpots(object):
             def __init__(self, indexable, threshold= 1E7 ):
                 self.indexable = indexable
                 self.threshold = threshold
                 self.N = len( indexable  )
             def _get_mask(self ):
                 mask = np.ones_like( np.array( self.indexable[0])    )
                 for key in range(self.N):
                     data = np.array( self.indexable[key])  #.copy()
                     badp = np.where(  data >= self.threshold )
                     if len(badp[0])!=0:
                         mask[badp] = 0
                 return mask
```

```
In [13]: class Masker(object):
             def __init__(self, indexable, mask):
                 self.indexable = indexable
                 self.mask = mask
             def __getitem__(self, key):
                 return self.indexable[key] * mask
```

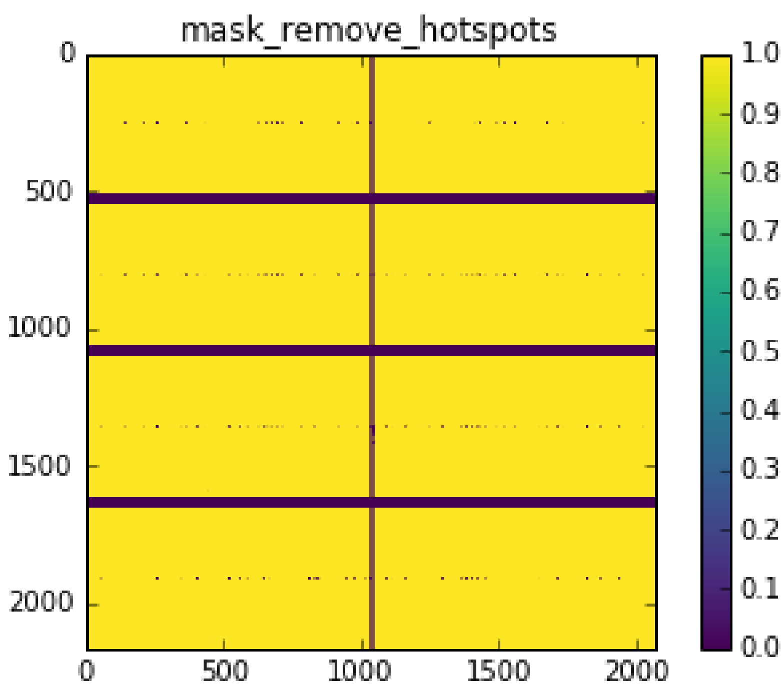
3 remove hotspots

```
In [14]: mask_rh  = RemoveHotSpots( imgs, 5E4)._get_mask()
```

```
In [15]: #%matplotlib notebook
```

```
In [16]: fig, ax = plt.subplots()
         im = ax.imshow(mask_rh , vmin=0,vmax=1,cmap='viridis')
         ax.set_title( 'mask_remove_hotspots')
         plt.colorbar( im  )
```

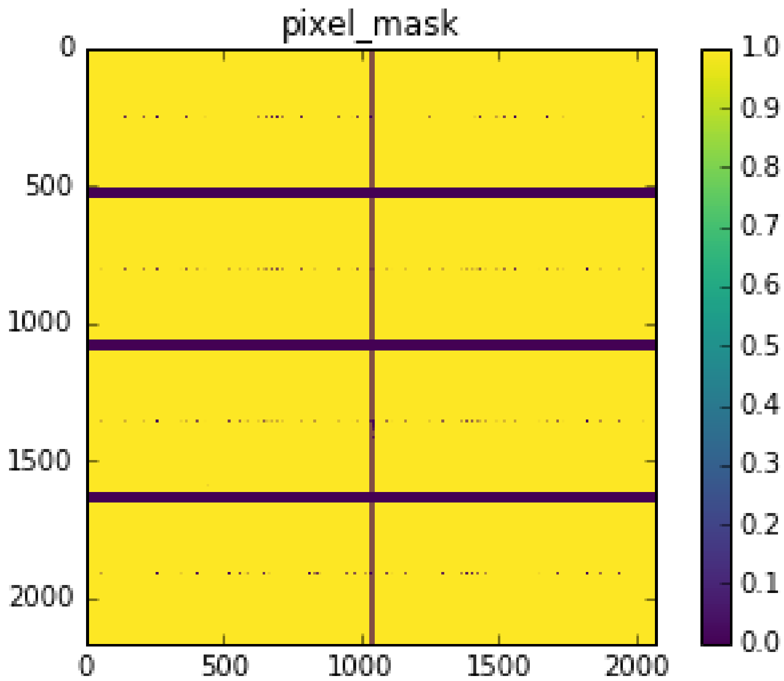
```
Out[16]: <matplotlib.colorbar.Colorbar at 0x7fe593d24668>
```



3.0.3 show pixel mask from data

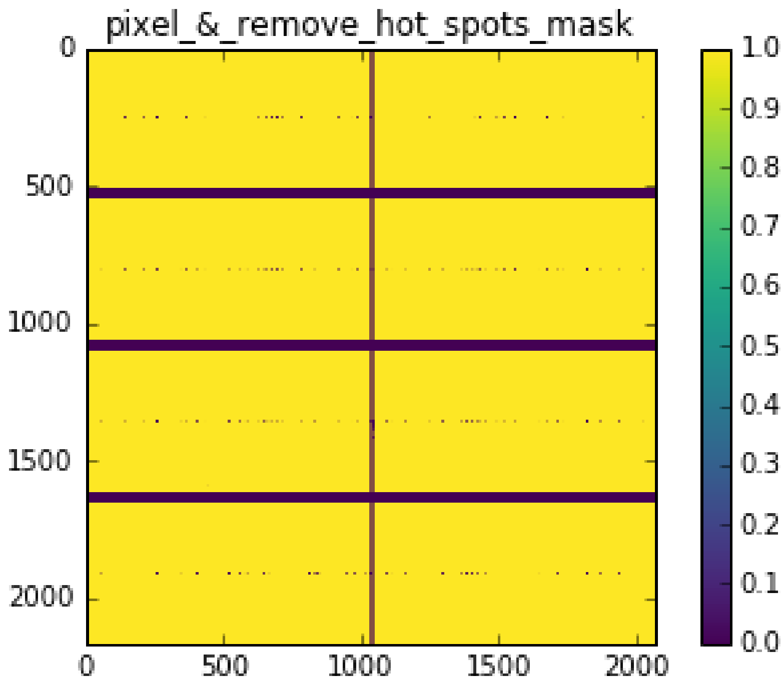
```
In [17]: #%matplotlib inline

         fig, ax = plt.subplots()
         im = ax.imshow(imgs.md['pixel_mask'], vmin=0,vmax=1,cmap='viridis')
         ax.set_title( 'pixel_mask')
         plt.colorbar( im )
```

Out[17]: <matplotlib.colorbar.Colorbar at 0x7fe593c20780>




```
In [18]: imgs_mask =   mask_rh * imgs.md['pixel_mask']
         fig, ax = plt.subplots()
         im = ax.imshow(imgs_mask, vmin=0,vmax=1,cmap='viridis')
         ax.set_title( 'pixel_&_remove_hot_spots_mask')
         plt.colorbar( im )
```

Out[18]: <matplotlib.colorbar.Colorbar at 0x7fe593b5c0b8>

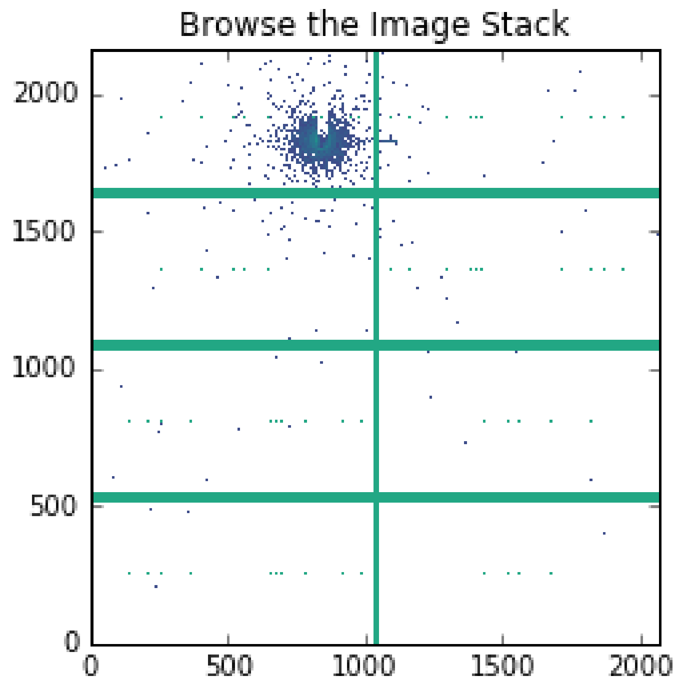


3.1 Interactive way to browse through images.

3.1.1 Note : Provide the number of images that you want to browse

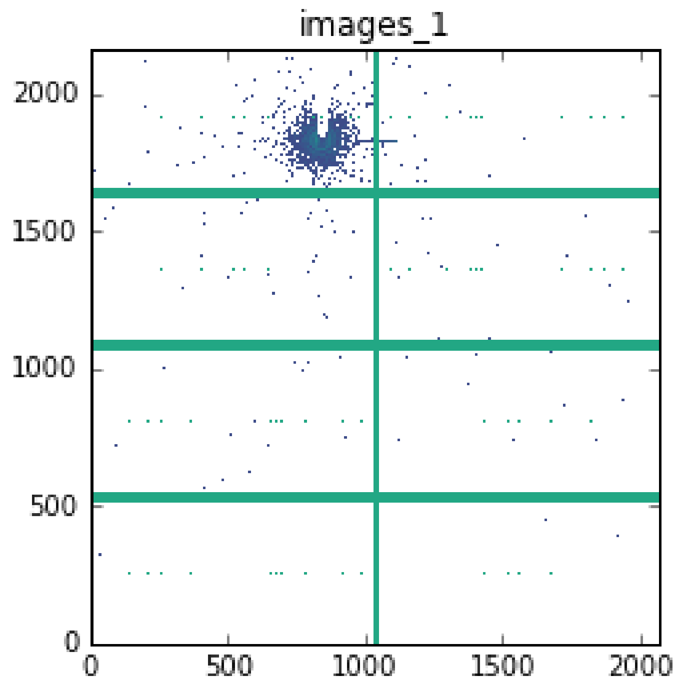
In [19]:
```
#%matplotlib inline
## there is a bug for %matplotlib notebook
from ipywidgets import interact

def view_image(i):
    fig, ax = plt.subplots()
    ax.imshow(imgs[i], interpolation='nearest', cmap='viridis',
                origin='lower', norm= LogNorm( vmin=0.001, vmax=1e10 ) )
    ax.set_title("Browse the Image Stack")
    #plt.show()

interact(view_image, i=(0, Nimg-1))
```

Out[19]:
```
<function __main__.view_image>
```



4 a movie of images

In [20]:
```
import time
def view_image(sleeps=1, ims=0, ime = 1):
    fig, ax = plt.subplots()
    for i in range( ims, ime  ):
        ax.imshow(imgs[i],  interpolation='nearest', cmap='viridis',
                    origin='lower', norm= LogNorm( vmin=0.001, vmax=1e10 ) )
        ax.set_title("images_%s"%i)
        time.sleep( sleeps )
        plt.draw()

view_image( .2, 0, 2)
```

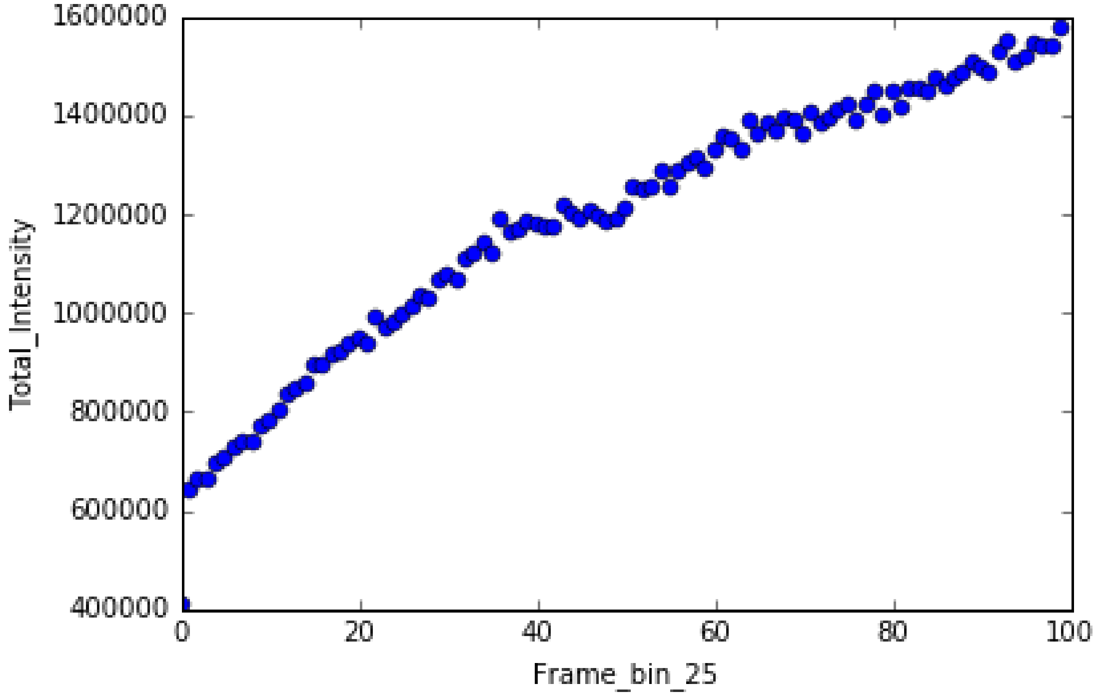


4.0.2 Get the Averaged Image Data

In [21]:
```
#hey, let's see if any images are bad!
bin_img =25
imgsum = [np.sum(img *imgs_mask) for img in imgs[::bin_img ]]
```

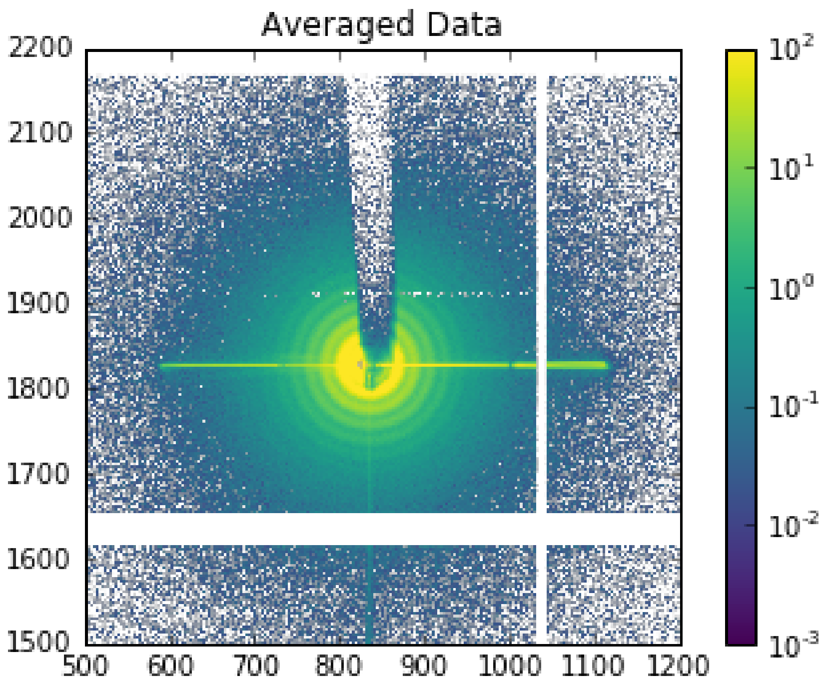
In [22]:
```
#%matplotlib inline
fig, ax = plt.subplots()
ax.plot(imgsum,'bo')
ax.set_xlabel( 'Frame_bin_%s'%bin_img )
ax.set_ylabel( 'Total_Intensity' )
```

Out[22]: <matplotlib.text.Text at 0x7fe593b04160>




```
In [23]: avg_img = np.average(imgs[::50], axis=0) * imgs_mask
```

```
In [24]: # Plot the result
         fig, ax = plt.subplots()
         im = ax.imshow(avg_img,  cmap='viridis',origin='lower', norm= LogNorm( vmin=0.001, vmax=1e2 )
         ax.set_xlim([500,1200])
         ax.set_ylim([1500,2200])
         fig.colorbar(im)
         ax.set_title("Averaged Data")
         plt.show()
```



4.1 Import all the required packages for Data Analysis

- scikit-xray - data analysis tools for X-ray science
  - https://github.com/scikit-xray/scikit-xray
- xray-vision - plotting helper functions for X-ray science
  - https://github.com/Nikea/xray-vision

In [25]:
```
import xray_vision
import xray_vision.mpl_plotting as mpl_plot
from xray_vision.mpl_plotting import speckle
from xray_vision.mask.manual_mask import ManualMask

import skxray.core.roi as roi

import skxray.core.correlation as corr
import skxray.core.utils as utils
```

```
/home/yuzhang/.conda/envs/user_analysis/lib/python3.4/site-packages/IPython/html.py:14: ShimWarning: The
  "`IPython.html.widgets` has moved to `ipywidgets`.", ShimWarning)
```

4.2 Note: Enter the following experiment information

- The physical size of the pixels
- Wavelegth of the X-rays - (units in Angstroms)
- Detector to sample distance
- Exposure time - (units in seconds)
- acqusition period - (units in seconds)

- dead time - (units in seconds)
- time per frame = (exposure time + dead_time or acqusition period) - (units in seconds)

In [26]:
```
imgs.md
```

Out[26]:
```
{'beam_center_x': 840.0,
 'beam_center_y': 336.0,
 'count_time': 0.0049999999,
 'detector_distance': 4.8400002,
 'frame_time': 0.00501,
 'framerate': 199.60079982206346,
 'incident_wavelength': 1.3794414,
 'pixel_mask': array([[1, 1, 1, ..., 1, 1, 0],
        [1, 1, 1, ..., 1, 1, 1],
        [1, 1, 1, ..., 1, 1, 1],
        ...,
        [1, 1, 1, ..., 1, 1, 1],
        [1, 1, 1, ..., 1, 1, 1],
        [1, 1, 1, ..., 1, 1, 1]], dtype=uint32),
 'x_pixel_size': 7.5000004e-05,
 'y_pixel_size': 7.5000004e-05}
```

In [27]:
```
# The physical size of the pixels
dpix = imgs.md['x_pixel_size'] * 1000.
lambda_ = imgs.md['incident_wavelength']    # wavelegth of the X-rays in Angstroms
Ldet = 5000.        # detector to sample distance (mm)

exposuretime= imgs.md['count_time']
acquisition_period = imgs.md['frame_time']

# deadtime= 0   # 60e-6
# timeperframe = exposuretime + deadtime
timeperframe = acquisition_period
```

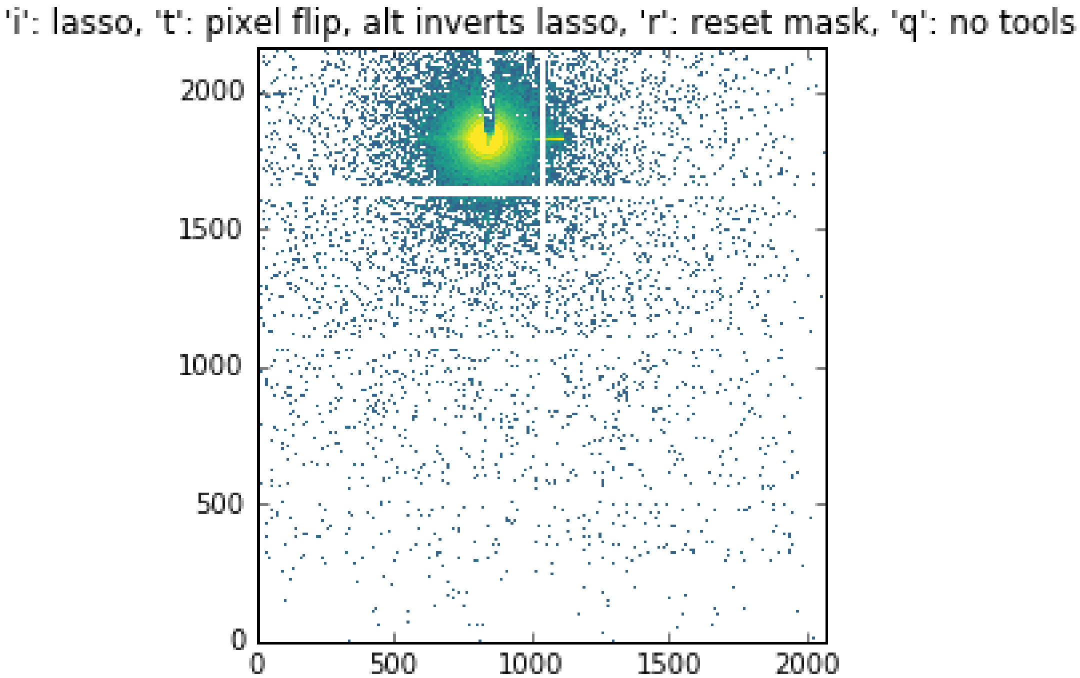
In [28]:
```
print (timeperframe)
print (exposuretime)
```

```
0.00501
0.005
```

4.3 Create the mask file

More information : https://github.com/Nikea/xray-vision/blob/master/xray_vision/mask/manual_mask.py

In [29]:
```
fig, ax = plt.subplots()
m = ManualMask(ax, avg_img,  cmap='viridis',origin='lower', norm= LogNorm( vmin=0.001, vmax=1e
```

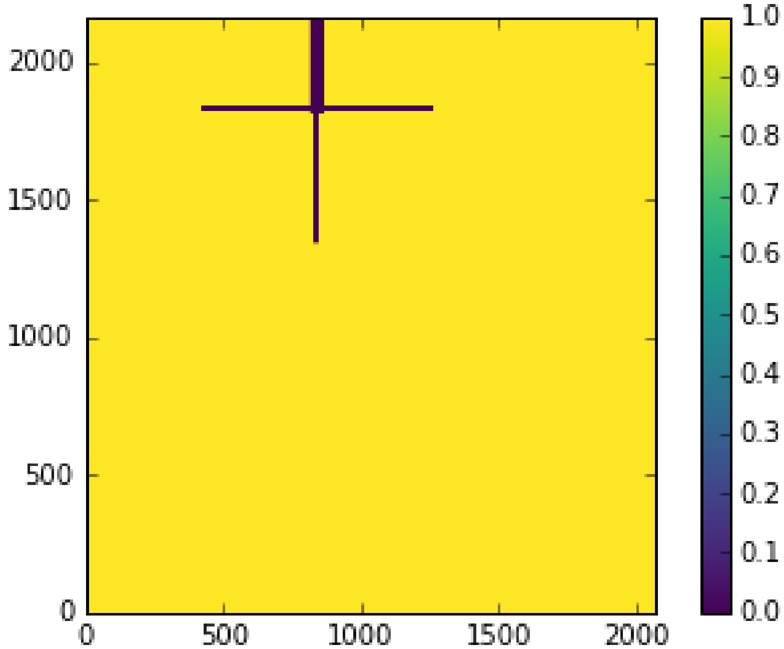


4.3.1 load a mask if exist

In [30]:
```
new_mask = np.load( '/XF11ID/analysis/Analysis_Pipelines/mask_Si.npy')
```

In [31]:
```
#new_mask = m.mask
fig, ax = plt.subplots()
im=ax.imshow(1-new_mask,origin='lower' ,vmin=0,vmax=1,cmap='viridis')
plt.colorbar( im )
```

Out[31]: <matplotlib.colorbar.Colorbar at 0x7fe5886ce048>

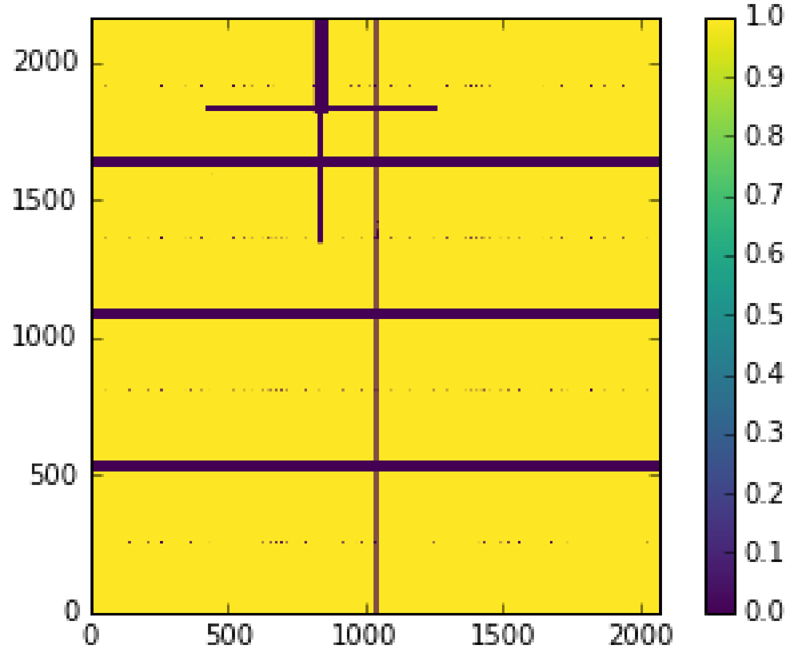


4.3.2 Combine the hand-drawn mask and the pixel mask

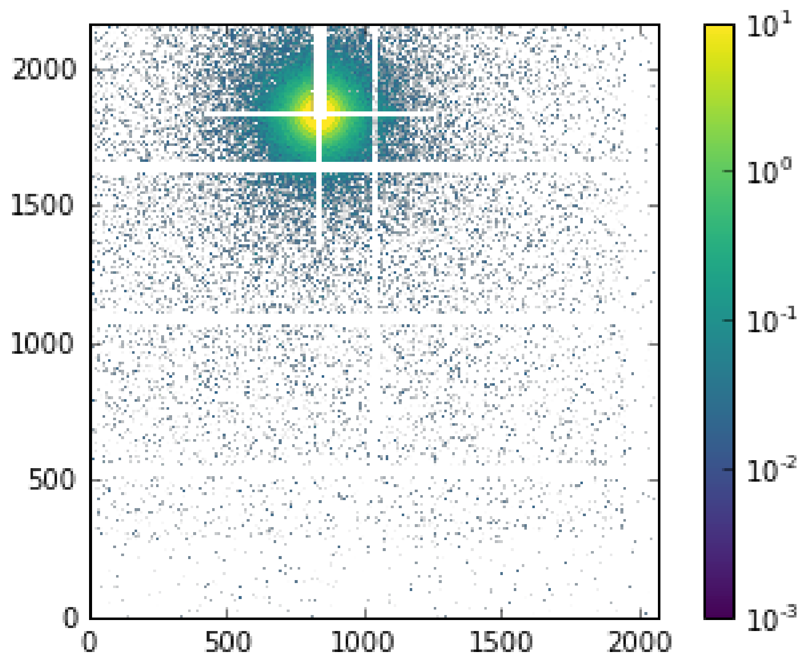
In [32]:
```
mask = (1-new_mask) * imgs_mask
```

In [33]:
```
fig, ax = plt.subplots()
im=ax.imshow(mask,origin='lower' ,vmin=0,vmax=1,cmap='viridis')
fig.colorbar( im )
```

Out[33]:
```
<matplotlib.colorbar.Colorbar at 0x7fe5817ab160>
```




```
In [34]: img_mask = avg_img * mask

         #%matplotlib notebook
         fig, ax = plt.subplots()
         im = ax.imshow(img_mask, cmap='viridis',origin='lower', norm= LogNorm( vmin=0.001, vmax=1e1 ) )
         fig.colorbar( im )

Out[34]: <matplotlib.colorbar.Colorbar at 0x7fe5816f0898>
```



4.4 Get the approximate center and see the statistic to make sure

In [35]:
```
#center = (1634.66, 838.6)  # center of the speckle pattern
#center = (imgs.md['beam_center_x'], imgs.md['beam_center_y'])
center = [840, 1830]

center
```

Out[35]: [840, 1830]

In [36]:
```
center=[center[1],center[0]]
#center=[center[0],center[1]]
```

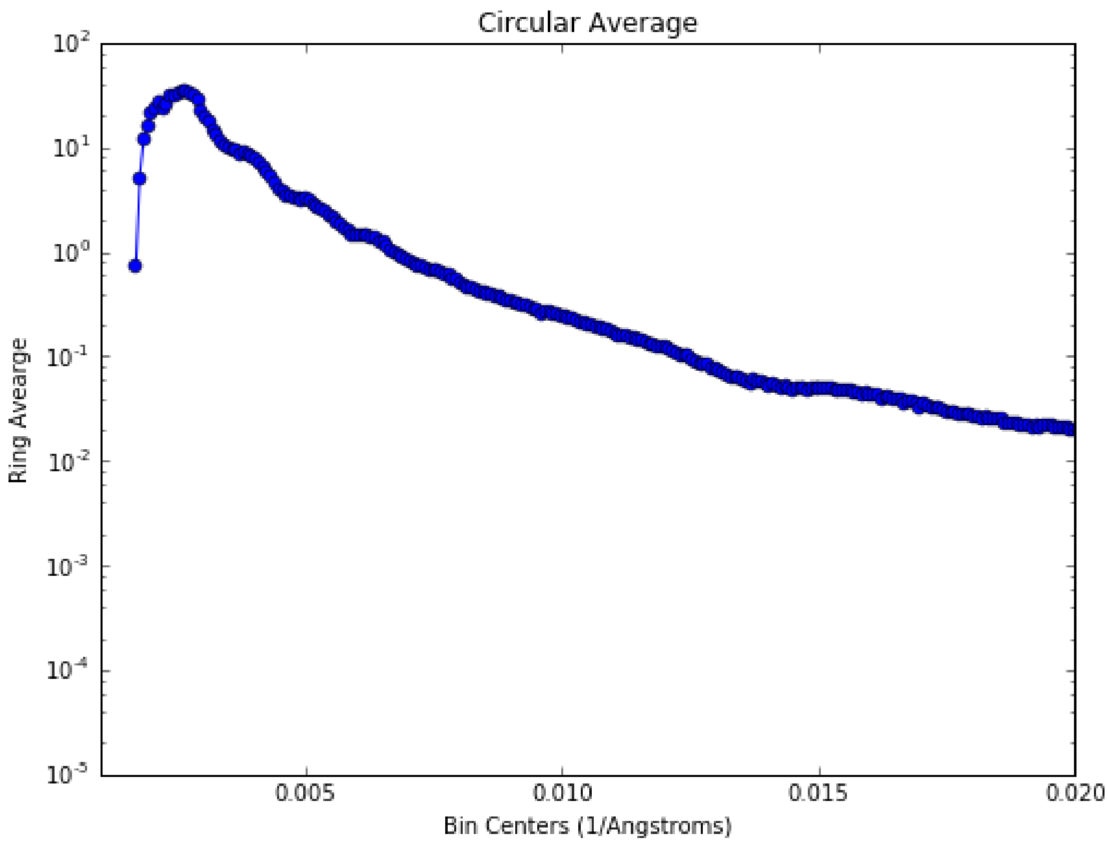
In [37]:
```
imgs.md['beam_center_x'], imgs.md['beam_center_y']
```

Out[37]: (840.0, 336.0)

4.4.1 Circular Average : compute the radial integartion from the center of the speckle pattern

In [38]:
```
bin_centers, ring_averages= roi.circular_average(img_mask,
        center, threshold=0, nx=2000, pixel_size=(dpix, dpix))

#  convert to q (reciprocal space)
two_theta = utils.radius_to_twotheta(Ldet, bin_centers)
q_val = utils.twotheta_to_q(two_theta, lambda_)
```

In [39]:
```
fig,axes = plt.subplots(figsize=(8, 6))
axes.semilogy(q_val, ring_averages, '-o')

#axes.plot(q_val, ring_averages, '-o')
axes.set_title("Circular Average")
axes.set_ylabel("Ring Avearge")
axes.set_xlabel("Bin Centers (1/Angstroms)")
axes.set_xlim(0.001, 0.02)

plt.show()
```



4.5 Create label array (Q rings)

4.6 can we change the function of roi.ring_edges to give same values as make_qlist?

```
In [40]: inner_radius = 44  # radius of the first ring
         width = 2       # width of each ring
         spacing =  (119-44)/9-2    # no spacing between rings
         num_rings = 10   # number of rings

         #  find the edges of the required rings
         edges = roi.ring_edges(inner_radius, width, spacing, num_rings)
         edges
```

```
Out[40]: array([[  44.        ,   46.        ],
                [  52.33333333,   54.33333333],
                [  60.66666667,   62.66666667],
                [  69.        ,   71.        ],
                [  77.33333333,   79.33333333],
                [  85.66666667,   87.66666667],
                [  94.        ,   96.        ],
                [ 102.33333333,  104.33333333],
                [ 110.66666667,  112.66666667],
                [ 119.        ,  121.        ]])
```

```
In [41]: two_theta = utils.radius_to_twotheta(Ldet, edges*dpix)
         q_ring_val = utils.twotheta_to_q(two_theta, lambda_)

         q_ring_val
```

```
Out[41]: array([[ 0.00300622,  0.00314286],
                [ 0.00357558,  0.00371222],
                [ 0.00414494,  0.00428158],
                [ 0.0047143 ,  0.00485094],
                [ 0.00528365,  0.0054203 ],
                [ 0.00585301,  0.00598966],
                [ 0.00642237,  0.00655902],
                [ 0.00699173,  0.00712838],
                [ 0.00756109,  0.00769773],
                [ 0.00813045,  0.00826709]])
```

```
In [42]: q_ring_center = np.array( [(q_ring_val[i][0] + q_ring_val[i][1])/2 for
                                    i in range(num_rings)])
         q_ring_center
```

```
Out[42]: array([ 0.00307454,  0.0036439 ,  0.00421326,  0.00478262,  0.00535198,
                 0.00592134,  0.00649069,  0.00706005,  0.00762941,  0.00819877])
```

```
In [43]: rings = roi.rings(edges, center, avg_img.shape)

         ring_mask = rings*mask
```

```
In [44]: (q_ring_center/6.841437171805092e-05)[9]
```

```
Out[44]: 119.839854621893
```

4.7 Extract the labeled array

```
In [45]: ring_mask
```

```
Out[45]: array([[ 0.,  0.,  0., ...,  0.,  0.,  0.],
                [ 0.,  0.,  0., ...,  0.,  0.,  0.],
                [ 0.,  0.,  0., ...,  0.,  0.,  0.],
                ...,
                [ 0.,  0.,  0., ...,  0.,  0.,  0.],
                [ 0.,  0.,  0., ...,  0.,  0.,  0.],
                [ 0.,  0.,  0., ...,  0.,  0.,  0.]])
```

```
In [46]: labels, indices = roi.extract_label_indices(ring_mask)
```

```
In [47]: labels
```

```
Out[47]: array([ 10.,  10.,  10., ...,  10.,  10.,  10.])
```

```
In [48]: indices
```

```
Out[48]: array([3540544, 3540545, 3540546, ..., 4033224, 4033225, 4033226])
```

```
In [49]: nopr = np.bincount( np.array(labels, dtype=int) )[1:]
         nopr
```

```
Out[49]: array([ 328,  450,  576,  649,  788,  871,  971, 1089, 1186, 1290])
```

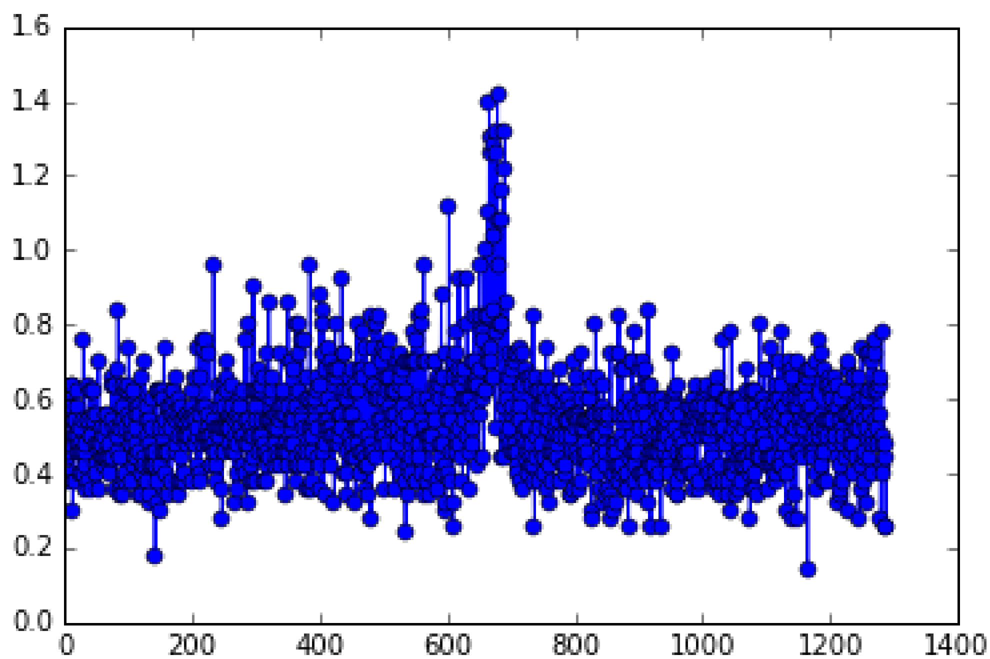
5 check center

5.1 this function should be changed,

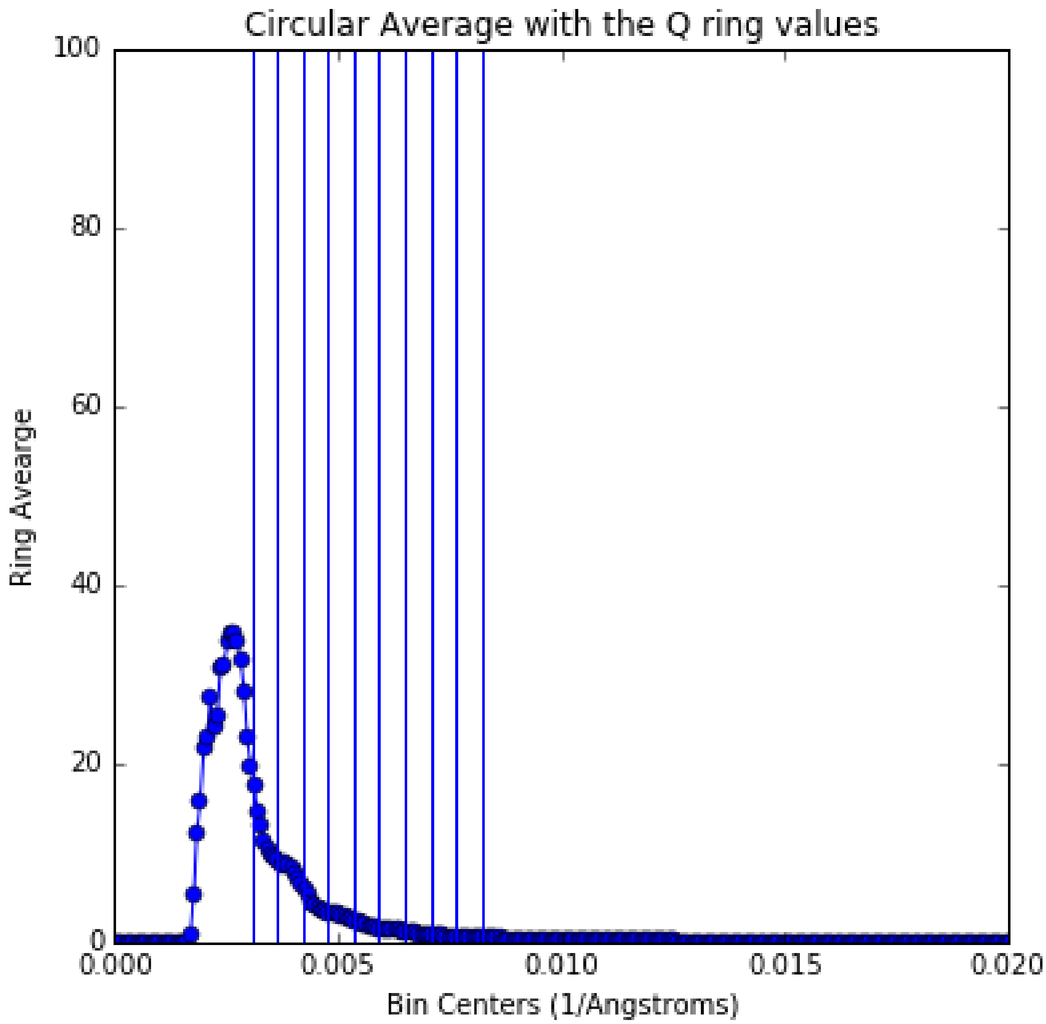
5.1.1 should check center befor given ring_mask

In [50]:
```
pixel = roi.roi_pixel_values( avg_img*mask, ring_mask, [10] )
fig,ax=plt.subplots()
ax.plot( pixel[0][0] ,'bo', ls='-' )
```

Out[50]:
```
[<matplotlib.lines.Line2D at 0x7fe581588898>]
```

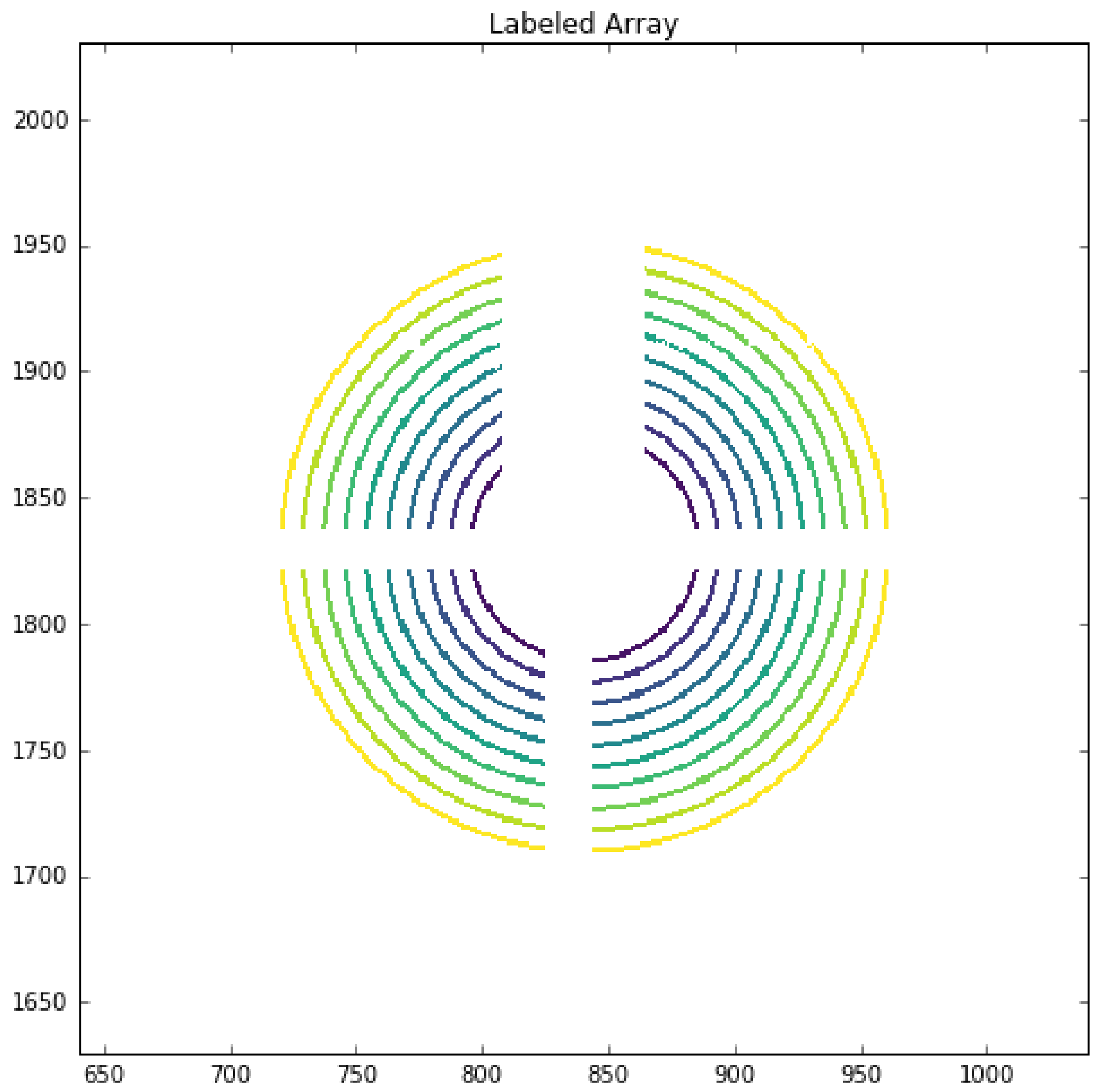


In [51]:
```
fig, axes = plt.subplots( figsize=(6, 6))
#axes.semilogy(q_val, ring_averages, '-o')

axes.plot(q_val, ring_averages, '-o')
axes.set_title("Circular Average with the Q ring values")
axes.set_ylabel("Ring Avearge")
axes.set_xlabel("Bin Centers (1/Angstroms)")
axes.set_xlim(0, 0.02)
axes.set_ylim(0, 100)
for i in range(num_rings):
    #axes.axvline(q_ring_val[i, 0])
    axes.axvline(q_ring_center[i])
plt.show()
```



In [52]:
```
#% matplotlib notebook
# plot the figure
fig, axes = plt.subplots(figsize=(8,8))
axes.set_title("Labeled Array")
im = mpl_plot.show_label_array(axes, ring_mask, cmap='viridis',origin='lower')

rwidth = 200

x1,x2 = [center[1] - rwidth, center[1] + rwidth]
y1,y2 = [center[0] - rwidth, center[0] + rwidth]
axes.set_xlim( [x1,x2])
axes.set_ylim( [y1,y2])
```

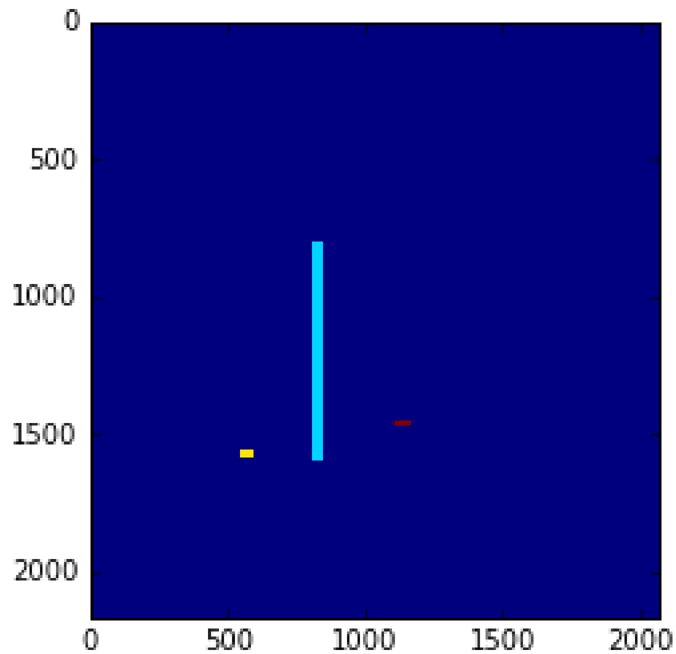
Out[52]: (1630, 2030)



5.2 Plot Kymograph (Waterfall plot) for a vertical and hortizontal cuts

Note : Give coordinates of the upper-left corner and width and height of each rectangle: e.g., [(x, y, w, h), (x, y, w, h)]

```
In [53]: vert_rect = ((800, 803,800, 40), (1554, 546, 30, 40), (1454, 1098, 20, 60))

         V_K_label_array = roi.rectangles(vert_rect, avg_img.shape)
         plt.figure()
         plt.imshow(V_K_label_array)
         plt.show()
```




```
In [54]: center
```

```
Out[54]: [1830, 840]
```

```
In [55]: V_K_label_array
```

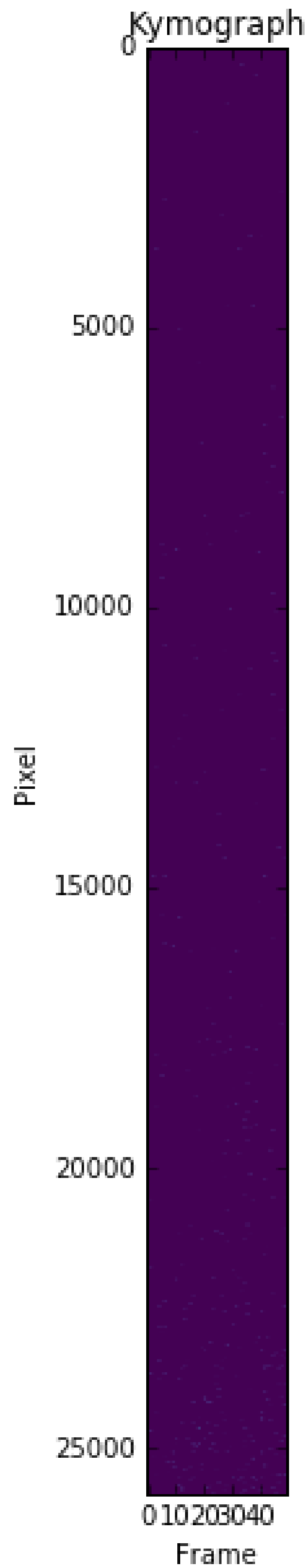
```
Out[55]: array([[0, 0, 0, ..., 0, 0, 0],
                [0, 0, 0, ..., 0, 0, 0],
                [0, 0, 0, ..., 0, 0, 0],
                ...,
                [0, 0, 0, ..., 0, 0, 0],
                [0, 0, 0, ..., 0, 0, 0],
                [0, 0, 0, ..., 0, 0, 0]])
```

5.3 Kymograph(waterfall plot) of the 3rd ring

```
In [56]: masker = Masker(imgs, mask)
```

```
In [57]: veri_kymo = roi.kymograph(masker[::50], V_K_label_array*mask, num = 1)
```

```
In [58]: fig, ax = plt.subplots(figsize=(14,10))
         ax.set_ylabel('Pixel')
         ax.set_xlabel('Frame')
         ax.set_title('Kymograph')

         im = ax.imshow(veri_kymo.T, cmap='viridis', vmax=10)
         #fig.colorbar( im   )
         ax.set_aspect(0.02)
         plt.show()
```


Kymograph
0
5000
10000
15000
20000
25000
Pixel
0 10 20 30 40
Frame

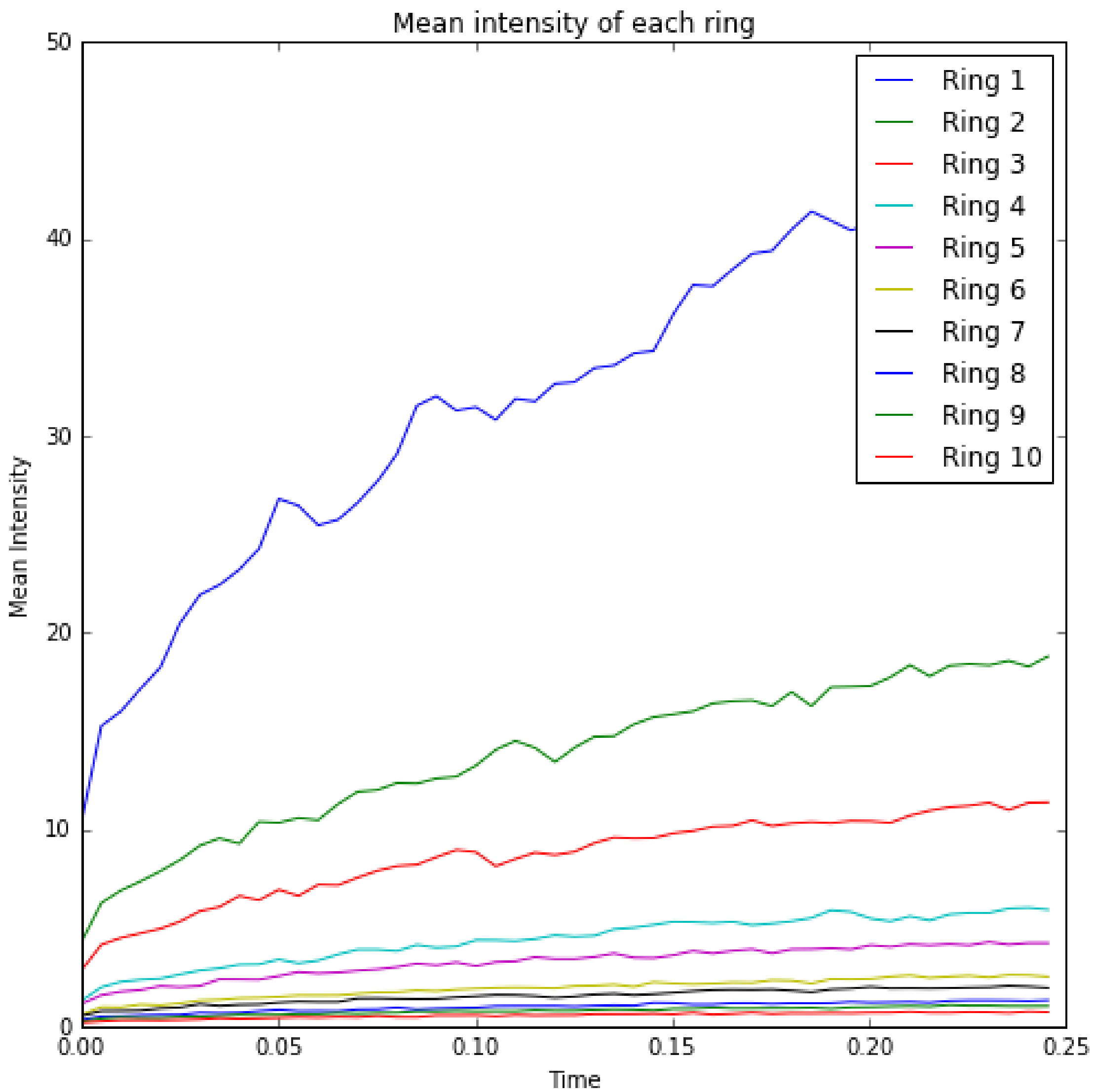
In [59]:
```
mask_data = masker[::50]  #this one is too slow if make  masker[::1]
mean_int_sets, index_list = roi.mean_intensity(mask_data, ring_mask)
```

5.4 Mean intensities for each ring

In [60]:
```
mean_int_sets.shape
```

Out[60]:
```
(50, 10)
```

In [61]:
```
time = np.arange(len(mask_data))*timeperframe  # get the time for each frame

%matplotlib inline
fig, ax = plt.subplots(figsize=(8, 8))
ax.set_title("Mean intensity of each ring")
for i in range(num_rings):
    ax.plot(time, mean_int_sets[:,i], label="Ring "+str(i+1))
    ax.set_xlabel("Time")
    ax.set_ylabel("Mean Intensity")
ax.legend()
plt.show()
```



In [ ]:

5.5 One time Correlation

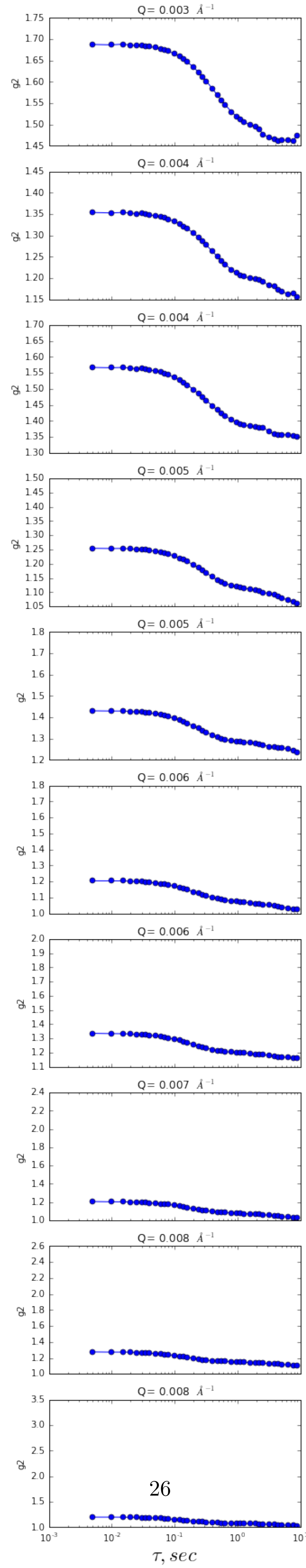
Note : Enter the number of levels and number of buffers for Muliti tau one time correlation number of buffers has to be even. More details in https://github.com/scikit-xray/scikit-xray/blob/master/skxray/core/correlation.py

```
In [62]: ring_mask = np.array( ring_mask, dtype=int)
```

```
In [63]: num_lev = 9
         num_buf = 8

         g2, lag_steps = corr.multi_tau_auto_corr(num_lev, num_buf, ring_mask,    imgs)
```

5.5.1 Plot the one time correlation functions

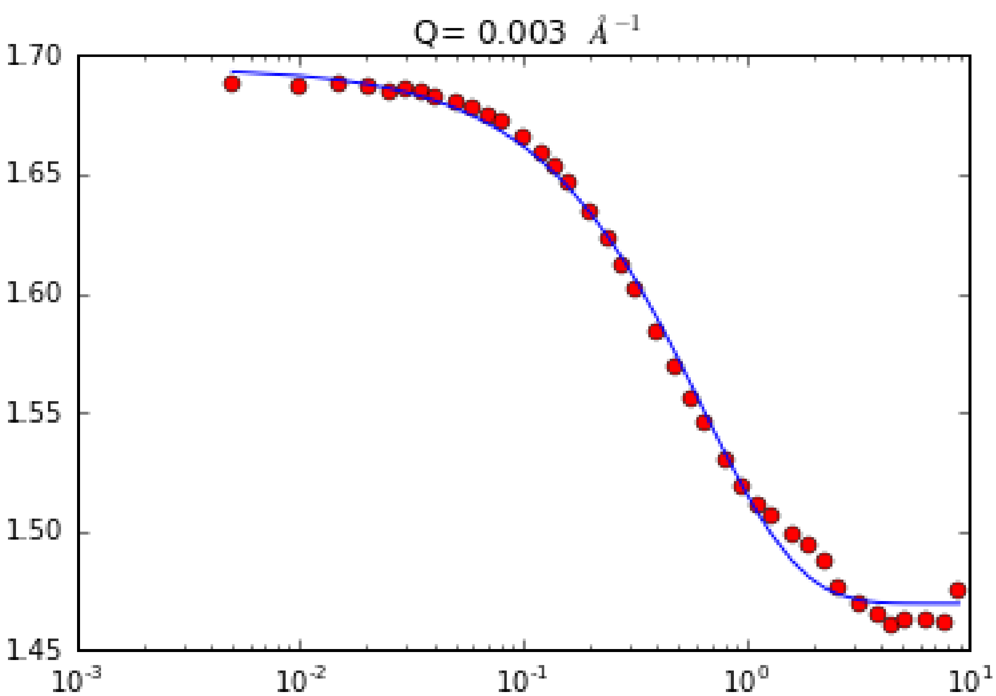
In [64]:
```
lags = lag_steps*timeperframe

fig, axes = plt.subplots(num_rings, sharex=True, figsize=(5, 30))
axes[num_rings-1].set_xlabel(r"$\tau,sec$", fontsize=22)
for i in range(num_rings):
    axes[i].set_ylabel("g2")
    axes[i].set_title(" Q= " + '%.3f  '%(q_ring_center[i]) + r'$\AA^{-1}$')
    axes[i].semilogx(lags, g2[:, i], '-o', markersize=6)
    #axes[i].set_ylim(bottom=1.10, top=1.15)
plt.show()
```

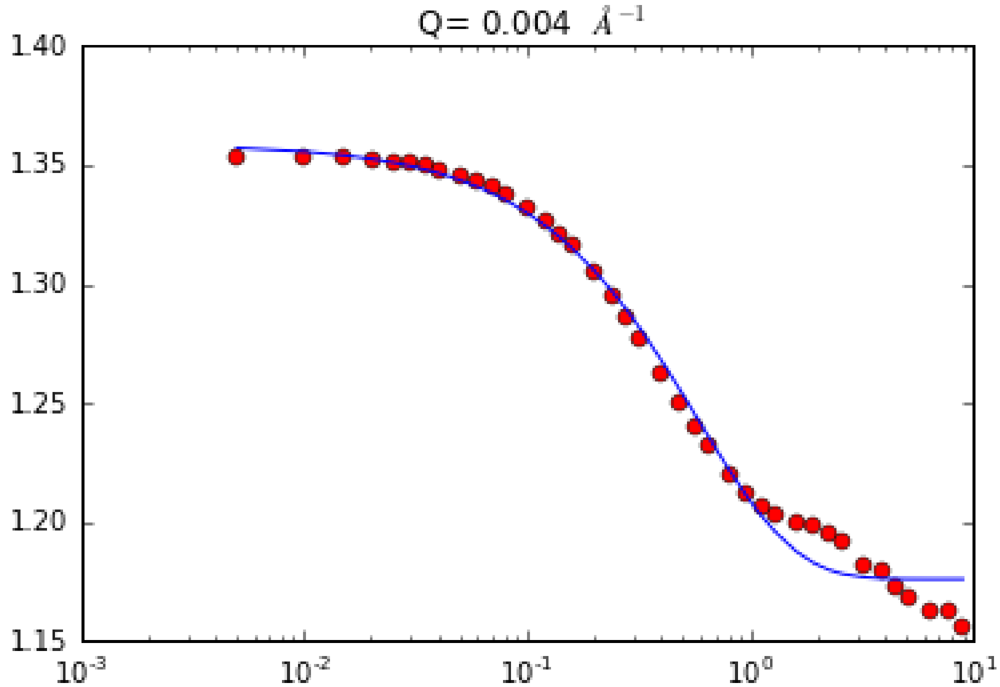

Q= 0.003 Å^{-1}
Q= 0.004 Å^{-1}
Q= 0.004 Å^{-1}
Q= 0.005 Å^{-1}
Q= 0.005 Å^{-1}
Q= 0.006 Å^{-1}
Q= 0.006 Å^{-1}
Q= 0.007 Å^{-1}
Q= 0.008 Å^{-1}
Q= 0.008 Å^{-1}
g2
10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1}
τ, sec

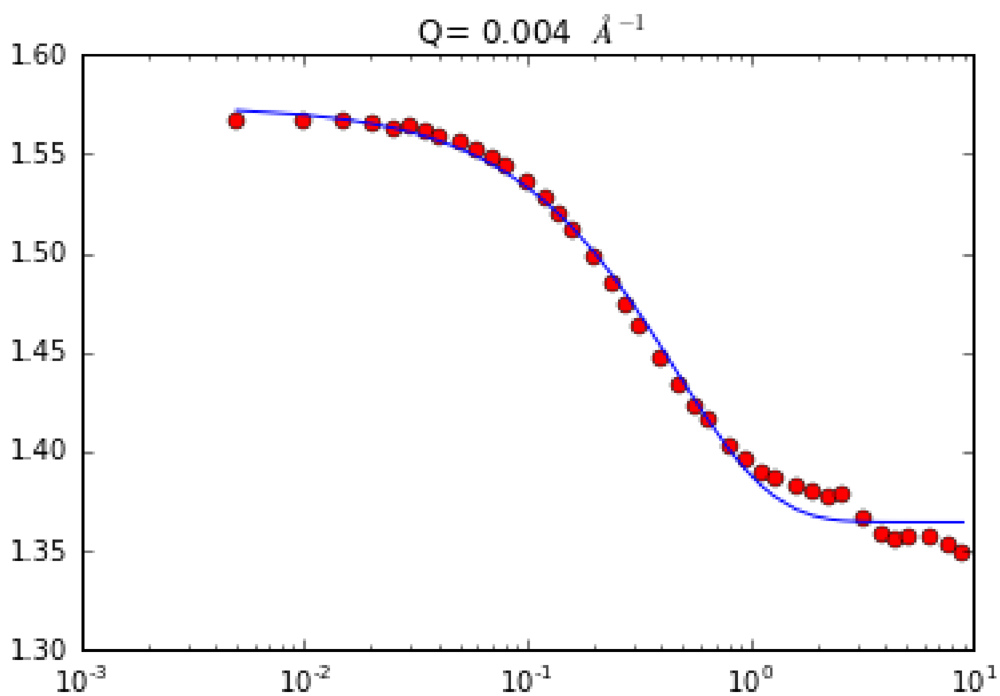
6 Fit g2

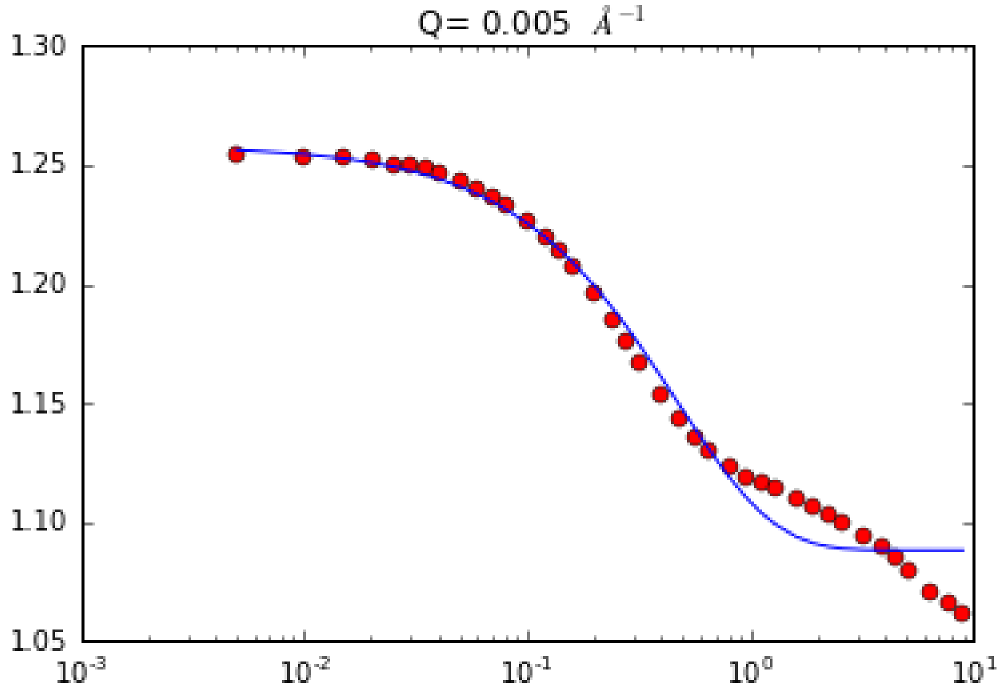
In [65]:
```
from lmfit import  Model
mod = Model(corr.auto_corr_scat_factor)
```

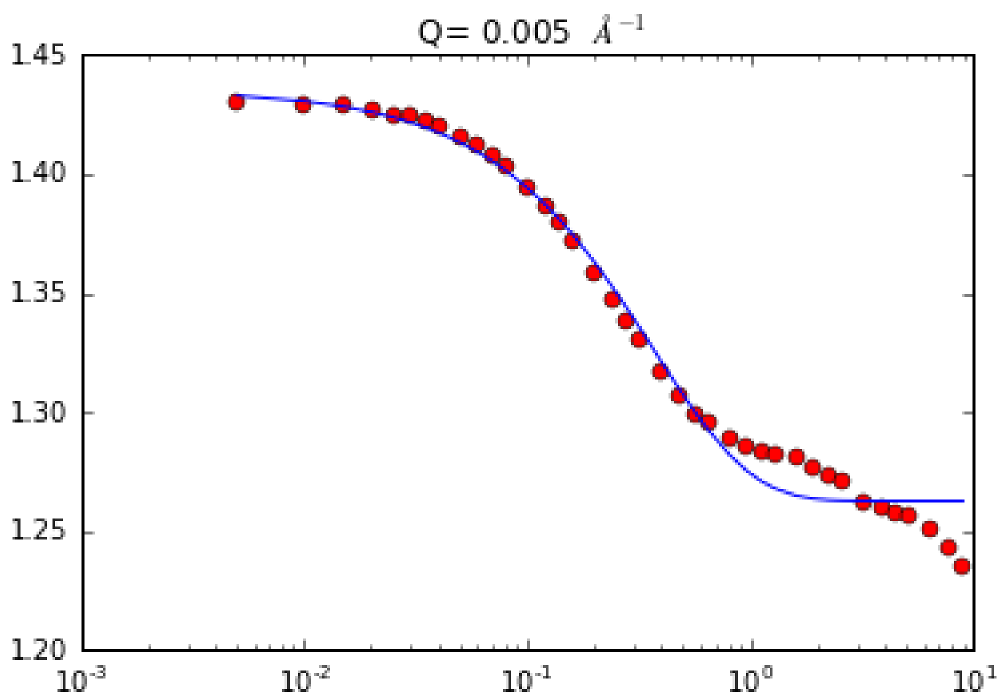
In [66]:
```
%matplotlib inline
rate = []
for i in range(num_rings):

    result1 = mod.fit(g2[1:,i], lags=lags[1:], beta=.1, relaxation_rate =.5,  baseline=1.0)

    rate.append(result1.best_values['relaxation_rate'])
    plt.figure()
    plt.semilogx(lags[1:], g2[1:, i], 'ro')
    plt.semilogx(lags[1:], result1.best_fit, '-b')
    #plt.ylim(1., 1.3)
    #axes[i].set_title(" Q= " + '%.3f  '%(q_ring_center[i]) + r'£\AA^{-1}£')

    plt.title(" Q= " + '%.3f  '%(q_ring_center[i]) + r'$\AA^{-1}$')
plt.show()
```

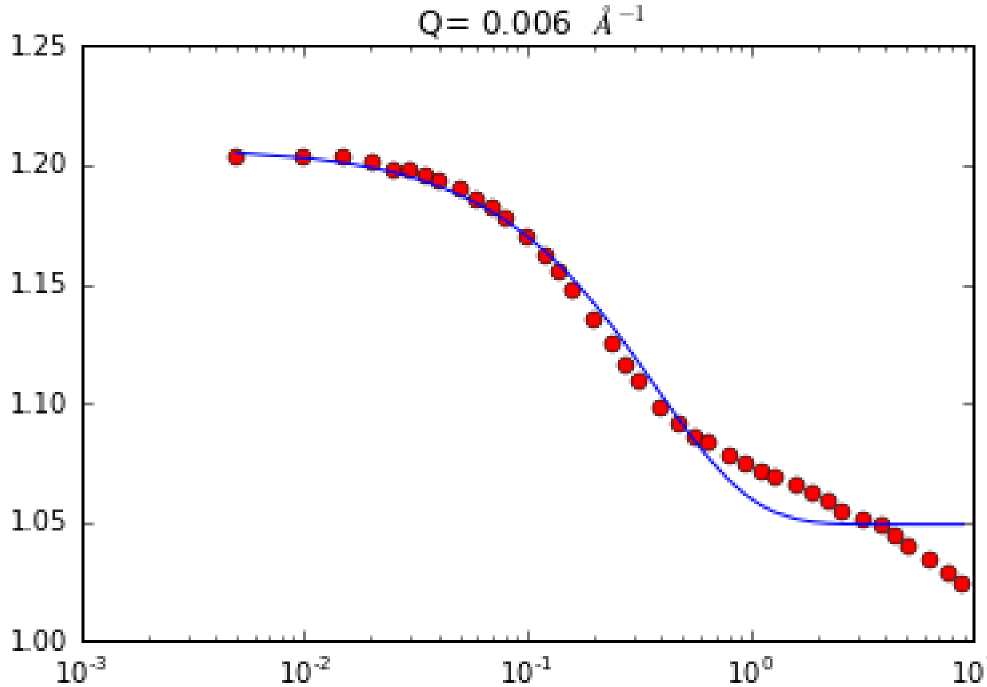


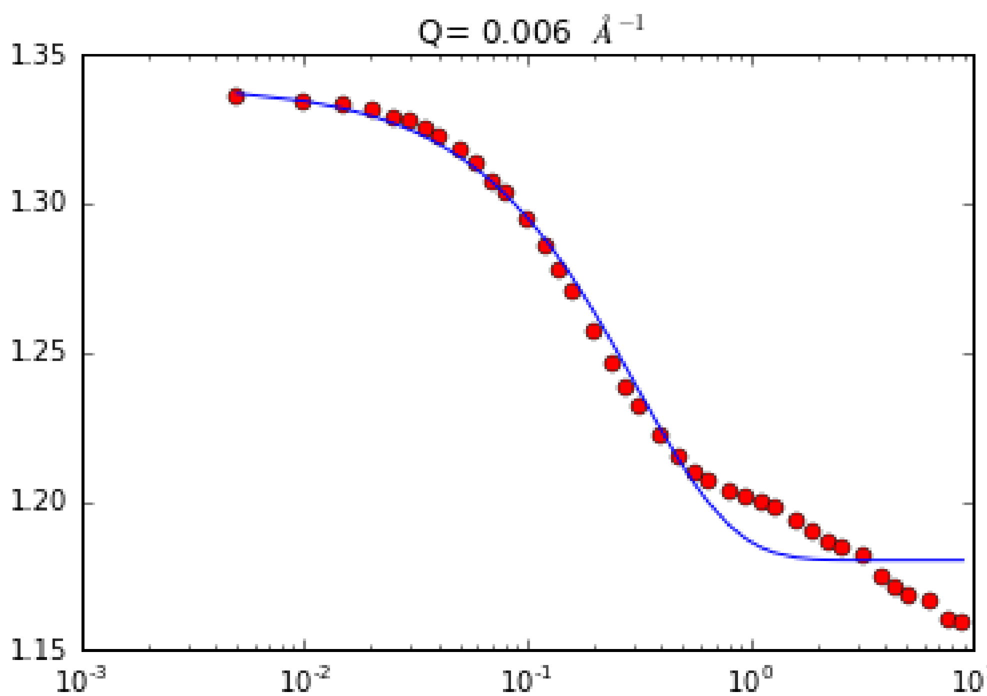

Q= 0.004 Å^{-1}
1.40
1.35
1.30
1.25
1.20
1.15
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}

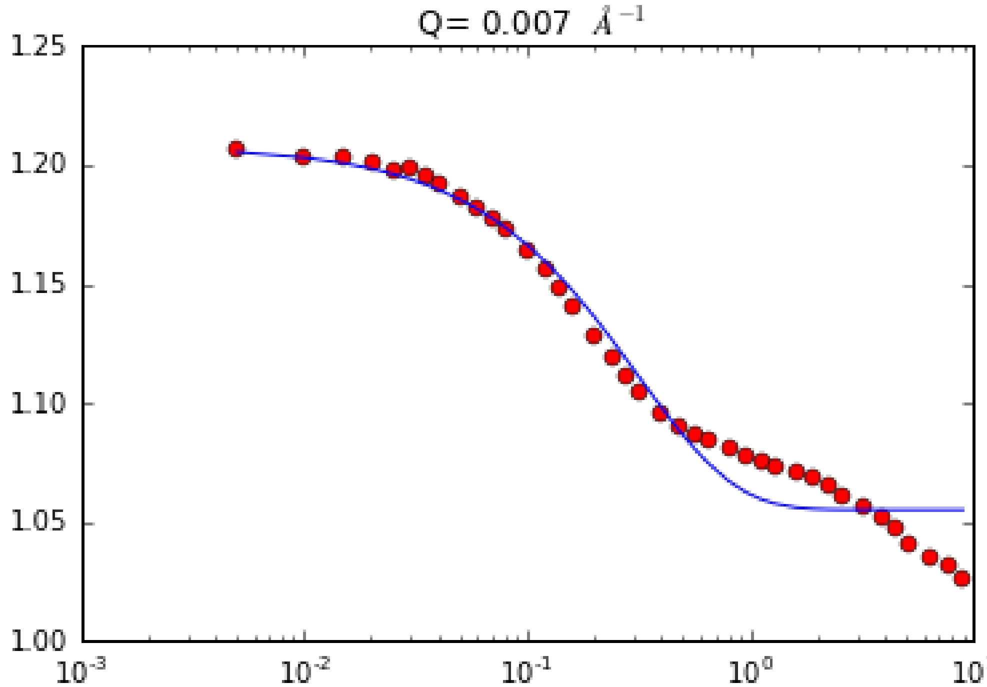

Q= 0.004 Å^{-1}
1.60
1.55
1.50
1.45
1.40
1.35
1.30
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}

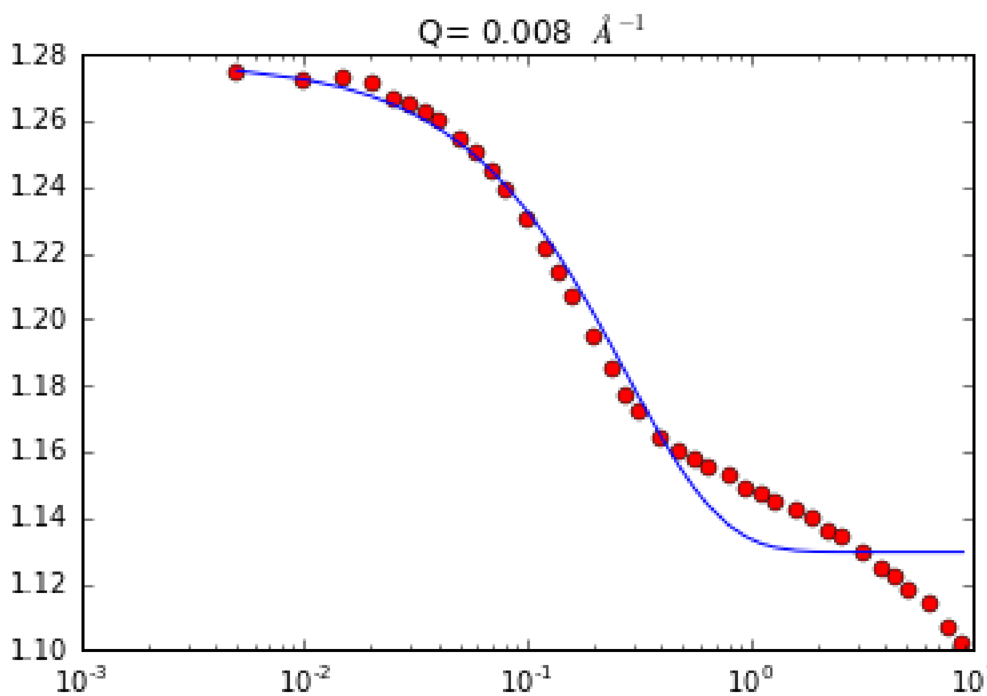

Q= 0.005 $\AA^{-1}$
1.30
1.25
1.20
1.15
1.10
1.05
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}

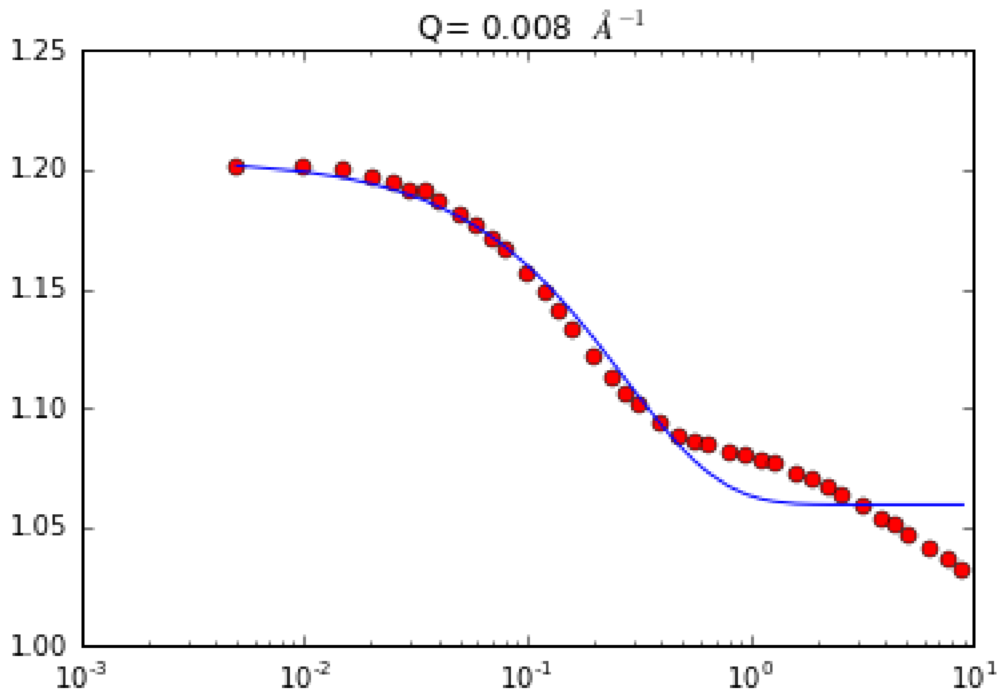

Q= 0.005 $\AA^{-1}$
1.45
1.40
1.35
1.30
1.25
1.20
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}


Q= 0.006 Å^{-1}
1.25
1.20
1.15
1.10
1.05
1.00
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}

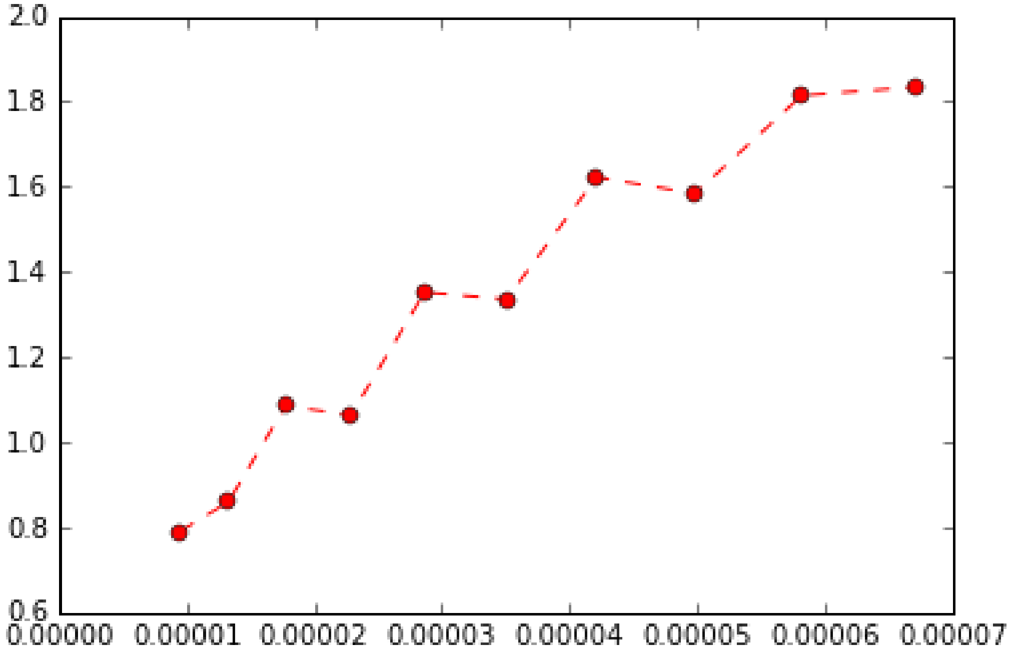

Q= 0.006 Å^{-1}
1.35
1.30
1.25
1.20
1.15
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}


Q= 0.007 Å^{-1}
1.25
1.20
1.15
1.10
1.05
1.00
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}


Q= 0.008 Å^{-1}
1.28
1.26
1.24
1.22
1.20
1.18
1.16
1.14
1.12
1.10
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}




```
In [67]: result1.best_values

Out[67]: {'baseline': 1.0594209410128113,
          'beta': 0.14492830189481173,
          'relaxation_rate': 1.8344361090851411}

In [68]: fig,ax=plt.subplots()
         ax.plot( q_ring_center**2, rate, 'ro', ls='--')

Out[68]: [<matplotlib.lines.Line2D at 0x7fe580428470>]
```

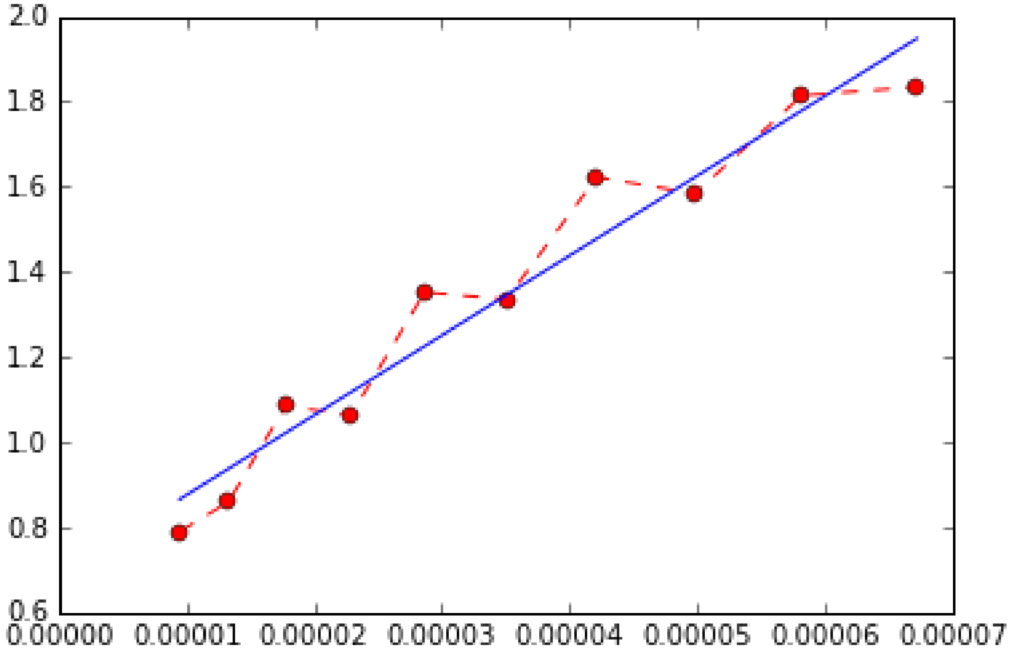



```
In [71]: D0 = np.polyfit(q_ring_center**2, rate, 1)
         gmfit = np.poly1d(D0)
         print ('The fitted diffusion coefficient D0 is:  %.2E   A^2S-1'%D0[0])
```

```
The fitted diffusion coefficient D0 is:  1.87E+04   A^2S-1
```

```
In [72]: fig,ax=plt.subplots()
         ax.plot( q_ring_center**2, rate, 'ro', ls='--')
         ax.plot( q_ring_center**2,  gmfit( q_ring_center**2),  ls='-')
```

```
Out[72]: [<matplotlib.lines.Line2D at 0x7fe58021f128>]
```



2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.00000
0.00001
0.00002
0.00003
0.00004
0.00005
0.00006
0.00007


```
In [ ]:
```