SAXS and GISAXS Techniques at beamline BW4:

Beamline Set up, Measurement and Analysis of Colloidal Crystals

Nirawat Thammajak

Chiang Mai University, Thailand

Dr. Rainer Gehrke

Supervisor

HASYLAB Group, DESY Summer Student Program 2007

Preface

DESY Summer Student Program is a great research experience. My practice in IDL language for writing the SAXS analysis program is an interesting task and valuable being the background for further analysis studies. BW4 beamline is brilliant and composed with advanced technology components, which I could closely inspect the details during the set up and measurement. Many scientific suggestions and discussions under professional researcher's supervision are invaluable. The research atmosphere in HASYLAB, DESY prominently provides me the inspiration and challenge for the higher education and serious research in my chemistry field with application of these synchrotron techniques. In addition, friendship among summer students from different universities in many countries and research team collaboration are somewhat promising for future research networks.

ATTORNE OTTATO

(Mr. Nirawat Thammajak) ...14.../...09.../...07...

I hereby proclaim my approval of this DESY summer student 2007 report of Mr. Nirawat Thammajak.

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(Dr. Rainer Gehrke)

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SAXS and GISAXS Techniques at beamline BW4: Beamline Set up,

Measurement and Analysis of Colloidal Crystals

Nirawat Thammajak^{*a*}, Rainer Gehrke^{*b*}

^a Summer student; Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

^b Supervisor; HASYLAB, DESY, Notkestrasse 85, D-22607 Hamburg, Germany

Abstract

Small angle x-ray scattering (SAXS) and grazing incidence small angle x-ray scattering (GISAXS) are very powerful tools for materials science. During this summer student program, I have practiced in the beamline set up and studied these techniques to characterize the structure of thin polymer films. The "Interactive Data Language (IDL)" was used to write the special analysis computer program for SAXS data, whereas the common data handling program "Fit2D" (http://www.esrf.eu /computing/scientific/FIT2D/) was used for GISAXS data evaluation. It is revealed that the structural arrangement of opal film samples shows two separate regions, lateral ordering near the surfaces and isotropic disorder in the bulk. Concerning the distances between particles in the bulk of each sample, it was figured out that the interparticle distance becomes smaller with decreasing wavelength of the corresponding opalescence wavelength of the samples. The same dependence could be shown for the particles at the surface which exhibit orientational ordering in addition. Furthermore, an expression for the geometrical corrections of SAXS-Data obtained at different center of primary beam incidence was derived and verified using experimental data.

1. Introduction to SAXS/GISAXS at beamline BW4

The beamline BW4 at the DORIS III storage ring at HASYLAB has been designed as a small-angle x-ray scattering instrument. Due to its wiggler generated beam with high flux and excellent collimation, analysis of this scattering data provides the structural information with very high resolution.



Figure 1. Schematic SAXS Apparatus

The SAXS/GISAXS instrument is total 56 meters in length, the longest beamline in HASYLAB. As sketched in Figure 1, the x-ray beam is produced by a wiggler and passes through the tilt absorber, which is capable to absorb the total power of the white wiggler beam. The beam is focused horizontally by a water cooled platinum coated silicon mirror with fixed cylindrical shape and is then monochromatized using a fixed exit double Si(111) crystal monochromater. It is followed by focusing the beam vertically using a plane mirror with a mirror bender, before the beam enters through a piezo-actuator controlled slit into the experimental hutch. Inside the 16 meters long hutch, the variable sample-detector distance can be changed between 1.8 and 12.7 m according to the desired resolution and the optical bench with the detector arrangement can be lifted and tilted by stepping motors to adapt to the GISAXS Scattering geometry. The primary beam intensity is monitored by ionization chambers with kapton windows. Before the beam can hit the detector, there is a beamstop mounted in the end-tube which is absolutely essential to prevent the primary beam from overloading and damaging the detector. Finally, a position sensitive two dimensional detector, MARCCD 165, is used to measure the scattered intensity. SAXS and GISAXS have many advantages that can be summarize as follows:

- It provides a non-destructive structural probe.
- It does not require special sample preparation which makes in-situ characterization possible.
- It yields excellent sampling statistics (averages over macroscopic regions).
- It provides information on nanometer scale.
- It provides information on particle geometry, size distributions, spatial correlations, etc.

In most typical experiments, the SAXS technique is performed in transmission geometry (Figure 2(a)). It extracts structural information on a length scale of about 0.5-600 nm and therefore can be promisingly applied for nano-structure materials, particle geometry and orientation of polymers and thin films, including in-situ experiments such as the investigation of temperature dependent mechanisms. In situations where transmission mode operation is not a feasible option, such as when the sample of interest is a thin film on a substrate or when only the surface microstructure is of interest, one must resort to using GISAXS, which uses grazing incidence reflection geometry to obtain surface and near surface sensitive x-ray scattering (Figure 2(b)). It is carried out at angles very near to the critical angle for total reflection, typical less than 1°. The penetration depth of the X-rays into the sample can be varied between a few nm and 1 mm, which allows for structural studies of very thin layers e.g. studies of semiconductor nanostructures (quantum dots, wires, and wells), studies of nano-composite thin films, studies of micro-domain formation, and ordering in thin films and surfaces of copolymer materials.



Figure 2. Schematic view of (a) SAXS and (b) GISAXS measurements and experimental images (Sources: http://people.ccmr.cornell.edu, www.esrf.eu)

2. Colloidal Crystal Sample

Monodispersed colloids of particles with identical size, shape, and interaction can spatially arrange themselves into the so-called "colloidal crystals" under the appropriate conditions. These periodic structures are distinguished from atomic/molecular crystals in that the individual particles do not have precisely identical internal arrangement. Their ordering is spontaneously adopted by the system through the thermal agitation or brownian motion of the particles. These conditions limit the sizes of particles which can form colloidal crystals to the range from about 0.01 to about 5 micrometers. The most spectacular evidence for the colloidal crystallization is the existence of natural opals, the fossilized remains of an earlier colloidal crystal suspension. The ideal opal structure is a periodic close-packed threedimensional array of silica microspheres with hydrated silica filling in the spaces which not occupied by particles.

Meanwhile, the periodic arrays of suspended colloidal particles of monodispersed silica or polymer spheres have attracted great interest for use as photonic crystals with potential applications in optics and optoelectronics. Colloidal crystals have been attempted to be produced from the synthetic monodisperse colloids such as suspensions of polymer microspheres. They have now become the important systems for the study of colloidal crystals and brought a strong requirement for detailed characterization of the internal structure. Here, SAXS and GISAXS techniques have shown to be the proper tools to analyse these colloidal crystals samples. In this study, polymer opal films in the opalescence which show blue, yellow, green and red colour, respectively, were characterized by both mentioned techniques. They are dispersions of rigid thermoplastic spheres, which have a coreshell architecture of polystyrene (PS), as a hard core particle, covered by poly(methyl

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methacrylate) (PMMA) and poly(ethyl acrylate) (PEA), as a second and third soft elastomeric shells, respectively, as shown in Figure 3.



Figure 3. Schematic of PS-PMMA-PEA core-shell polymer particle

For film formation, these core-shell particles were coagulated in methanol and then uniaxially compressed at 170°C between poly(ethylene terephthalate) (PET) foils, as shown in Figure 4. This process results in polymer opal films which behave as photonic crystals. Depending on the particle size in the initial dispersion, the films show different reflection colours, as mentioned above, ranging from blue (for "blau" sample) over green (for "gruen" sample) and yellow (for "gelb" sample) to red (for "rot" sample) if illuminated perpendicularly with white light. With SAXS measurement, one could observe a bulk order rearrangement of the particles inside a film, whereas, a lateral order near the film surface could be complementary revealed by GISAXS measurement.



Figure 4. The opal film fabrication by compression shear-assembly of PS-PMMA-PEA core-shell particles

3. SAXS Data Analysis by IDL based program

The SAXS data in transmission show two separate contributions: an isotropic from the bulk overlaid by anisotropic crystal like reflections from the highly oriented layers near the front and near surface. In order to separate the isotropic contribution the following strategy was used:

Starting at the beam center position, radial intensity cuts with subsequently increasing azimuthal angle were extracted from the 2D-pattern and all cuts were plotted over each other. At each scattering angle, the intensity in the various cuts must be either only caused by the isotropic contribution or is increased by additional anisotropic contribution. If one assumes, that each cut has certain regions which are only affected by the isotropic contribution taking for each scattering angle, the minimum of all corresponding intensities in the cuts will lead to a baseline curve, which represents the radial contribution from the isotropic part of the sample.

The sample was measured with different angles between the primary beam direction and the sample surface normal varying from perpendicular incidence to angles around 80°. The aim is to record the intensity contribution from the anisotropic part in a large fraction of reciprocal space. The intensity measurement has to be corrected for two geometrical effects, namely the increase of effective scattering volume and absorption with decreasing angle of incidence. After normalizing the data to primary beam intensity by means of the ionization chamber data, the integrals of the extracted baseline curves as function of the incidence angle should reflect this geometrical dependence.

SAXS data appear as continuous functions of scattering angle and are not straightforward for analysis. One will usually have to reduce this 2-D profile to a 1-D set of intensity vs. wave vector or angle data. Normally, programs like "Fit2D" can be used to analyze such data, however, it is important to put many required parameters and do it manually for each single scattering pattern e.g. to fit the experimental curve with a theoretical generated one. Using IDL (Interactive Data Language, Research Systems Inc.), a computer program was written to manage lots of data series and analyze each single pattern automatically. The schematic steps of IDL program for SAXS data analysis is shown in Figure 5.



Figure 5. Flowchart showing the analysis procedure of the IDL program

After getting ASCII files from the IDL program, they were finally analyzed using "Origin 7.5" scientific software. The ASCII file data of the baseline ($\mathbf{0}$) were

plotted to find the angular position of each order, to obtain the structural distance correlation information. In Figure 6, the extracted baseline was then directly generated from the corresponding minima of all radial intensity cuts.



Figure 6. The plot of radial scans and baseline extraction from minimum intensity

ASCII file data of integral (2) were used to generate a relation between an area under the baseline curve and the geometry of the measurement, from which one can deduce the influence of the scattering geometry on the relative scattering power. The detailed program can be found in appendix ii.

4. Experimental Procedures

SAXS and GISAXS measurements were conducted at the beamline BW4 during the exercise week. The operation steps can be summarized as follow.

1. Beamline Set Up

The optical bench in the hutch is partly removed and adapted in length and sample position. The length of some tubes can be changed easily by flipping 90° of a longer tube to be replaced by a shorter one. After all parts of the beam path were carefully connected, the height of the tube was adjusted in the proper position by stepping motors. The set up process for SAXS and GISAXS is similar in those described steps. It is different in the desired length of the flight tube and some components in each the individual measuring environment. It should be noted that, inclining the angle of the flight tube by 1° was done only for GISAXS. Basic set-up parameters important for each operation mode are shown in table 1.

Parameter	SAXS	GISAXS
Sample-to-detector distance	12.7 m	12 m
Photon energy	8.98 keV	8.98 keV
Wave length	0.138 nm	0.138 nm
Pixel size of CCD	79 µm	79 µm
Angle of incident beam	90°-20°	0.3°

Table1. The basic set-up parameters for SAXS and GISAXS

2. Beam alignment

After opening the beam shutter, the beam was observed by a digital camera for finding its position during the beam scan passing pieces of collagen horizontally (ydirection). The center position of the primary beam is adjusted under computer control before scanning of the slits, which were controlled by piezoactuator motors.

3. Sample Measurement

The sample was put on the sample holder and scanned in the y-direction for making the incident beam to hit on the sample, followed by the x-direction to make sure that the sample is flat and ready to be measured. The shutter must be closed before the CCD is used to detect the result of scattering. Sample measurement is started by supply the acquisition time by programming command and check the highest intensity before making a CCD recording of data which will not saturate the CCD camera. The measured scattering angles are in the range of 0-95° for SAXS and $0.30 - 0.45^{\circ}$ for GISAXS, respectively.

4. Data analysis

The IDL program was applied for SAXS data analysis. An easy command, for example, *test7*, *'blau'*, was typed to run the program for blau sample series characterization. Data processing by this program is necessary to be done in IDL environment, the computer screen during use of IDL is shown in Figure 7.



Figure 7. Computer screen showing the IDL program for SAXS analysis

After starting the program, it asks for the amount of data sets which will be processed, type "0" in case of all data. The first pattern will be displayed for finding the beam center interactively. At least 3 points of circular coordinates, which one could see on screen (Figure 8(a)), have to be clicked on with the mouse before pushing any key for further program processing. Figure 8(b) shows the radial scanning paths on a scattering pattern, the intensity distributions along these paths were then plotted one over the other as a function of s-value (Figure 8(c)). The baseline is directly generated from the corresponding minimum of all intensity curves in each single pattern which is then plotted (Figure 8(d)) and stored in an ASCII file. When all patterns in each series were completely proceeded, baseline curve areas which can be obtained by integration were calculated and plotted as a function of the angle between incident beam and sample surface before storing in ASCII file. These secondary data will be analyzed based on "plot and fit" by common scientific software "Origin7.5"

The GISAXS data, were extracted from scattering patterns by "Fit2D" program and were then plotted to see the order of scattering intensity.



Figure 8. Each step results gained during SAXS patterns analysis by the IDL writing program (a) finding beam center, (b) radial scanning of data, (c) overlaid plotting of scattered intensity versus s-value, and (d) plotting of extracted baseline.

5. Results and discussion

The scattering patterns, as shown in Figure 9, were obtained by using "Fit2D" program. These typical images were selected to show the different between SAXS and GISAXS scattering patterns. However, these are just only primary results which were then required for further analysis mentioned above.



Figure 9. Typical experimental images of (a) SAXS, and (b) GISAXS patterns

It can be seen in Figure 10 that the blau's baseline plot shows the intensity maxima correlated to order of s-values. These maxima were figured out to plot the order of s-values which shows the linear relation from the origin coordinates (Figure 11). For other colour polymer opals, the baseline curves are not shown here, they are all respected to linear correlation with the different slopes (Figure 12). The interpaticle distances (D) of each sample were disclosed by slopes, s-values, of each linear relation, when

$D = 1/s = 2\pi/q$

It is revealed that those interparticle distances of polymer opal films are distinguish and led to the different in reflection colours. Interparticle distance in blau sample is smaller than gelb, gruen, and rot samples, respectively, as shown in Table 2.



Figure 10. The example of blau's baseline plot showing order of maxima



Figure 11. The example of blau's order plot corresponded to the s-value shows high precision of linear relation



Figure 12. The s-value order plots of each sample which were used to characterize the interparticle spacing

Samples	\mathbb{R}^2	s (nm ⁻¹)	D _{SAXS} (nm)
Blau	0.99934	0.00623	160.5
Gelb	0.99925	0.00523	191.2
Gruen	0.99859	0.00504	198.4
Rot	0.99971	0.00443	225.7

Table 2. Linear regression and interpreted data of s-value order plots of each sample

By SAXS technique, one could observed that the scattering shows a contribution caused by strong distance correlation without orientational ordering, which is caused by the particles in-between the oriented layers on both sides. The measurements were carried out not only the perpendicular direction, but also investigated in other directions by goniometer rotation in range of 20° - 95° . Here, blau sample is studied, for example, in the influences of scattering geometry on the scattering intensity.



Figure 13. Schematic view of beam path area (A) when the beam passes the sample, where, d: sample thickness, b: beam size, β : measured angle.

From the second set of IDL derived ASCII files. Integral intensity plot shows the relation between areas under the baseline curves and beam position which preliminary gives information about the beam path area of scattering material (Figure13). Blau's film was decreasingly seen by the beam when it was measured at higher position of angle, as seen from Figure 14. Changes in that such integral intensity are useful in finding the scattering coefficient, μ , which is the characteristic parameter of each material. This curve was fit with the assumed geometrical relation derived according to Figure 13;

$$I = C(d*b/\sin\beta)exp(-\mu*d/\sin\beta) + D$$

where, I: Integral Intensity, μ : scattering coefficient, d: sample thickness, C and D: constants



Figure 14. The example of blau's integral plot as a function of the measured angles shows high precision of equation fitting

Fitting result of blau's integral plot showed corresponded relation in the above scattering equation. Unknown parameters of scattering coefficient (μ) and sample thickness (d) were finally disclosed to be 1.75 and 0.097, respectively. However, it is obvious that these two parameters are mainly appearing as a product in the equation which makes it impossible to fit each parameter separately with a sufficient degree of precision.

In addition, SAXS patterns also provide Bragg-like reflections which can be contributed to a regular arrangement of the particles near the film surface. The lateral distance correlations of this arrangement can be further characterized by GISAXS technique. Figure 15 shows the extracted data from GISAXS patterns. They contain the lateral information of each polymer opals' surface, which scarcely to be obtained by SAXS technique. With the same relation, $D = 1/s = 2\pi/q$, one can figure out the lateral distances of each samples in the near surface by q-value. As shown in Table 3, lateral distance between particles in gruen sample is smaller than in blau, gelb, and rot samples, respectively.



Figure 15. The GISAXS evaluation plots of each sample

q (nm ⁻¹)	D _{GISAXS} (nm)
0.0295	213.0
0.0264	238.0
0.0303	207.4
0.0237	265.1
	q (m) 0.0295 0.0264 0.0303 0.0237

Table 3. Interpreted data of q-values to the lateral distances (D_{GISAXS}) of each samples

6. Conclusions

By mean of SAXS measurement, it is demonstrated that opal film samples have a structural arrangement in two separation forms, the lateral ordering near the surface and isotropic disorder in the inner thick layer. The contributions of these structural formations can be seen from the SAXS patterns, which appeared both isotropic ring and Bragg-like reflections. Distances between bulk particles of each sample were figured out that blau has an interpaticle distance smaller than gelb, gruen, and rot samples, respectively. Verification of scattering geometry shows influence on scattering intensity which one can derive equation to explain and receive a product of important scattering parameters, $d^*\mu$. Whereas, GISAXS was conducted to investigate the distance correlations at surface. Gruen sample was observed that having lateral distance smaller than blau, gelb, and rot samples, respectively.

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Appendix	i
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Time Schedule

Activities	Week (25 July – 18 September)							
	1	2	3	4	5	6	7	8
1. Lectures attendances								
2. Writing the computer program (in IDL language) for Small Angle X-ray Scattering (SAXS) data analysis								
3. Practice in beamline set up and alignment for SAXS and GISAXS								
4. SAXS and GISAXS measurements								
5. Characterization of the measured scattering patterns								
6. Conclusion and report								

Appendix ii

IDL writing program for SAXS Data Analysis

@lsqCircleFit.pro @Read_key.pro :------

```
function load index, fname
openr,unit,fname,/get lun
n=0
buf="
repeat begin
    readf.unit.buf
    n=n+1
    endrep until eof(unit)
close,unit
free lun,unit
data={record,name:",pos:0.0,accutime:0.0,smflag:",idoris:0.0,igrid:0.0,ioni1:0.0,ioni2:0.0,ibea
mstop:0.0,dummy1:0.0,dummy2:0.0,dummy3:0.0}
data=replicate(data,n)
openr,unit,fname,/get lun
for i=0,n-1 do begin
       readf,unit,buf
       fields=strsplit(buf,',',/extract)
       data(i).name=fields(0)
       data(i).pos=float(fields(1))
       data(i).accutime=float(fields(2))
       data(i).smflag=fields(3)
       data(i).idoris=float(fields(4))
       data(i).igrid=float(fields(5))
       data(i).ioni1=float(fields(6))
       data(i).ioni2=float(fields(7))
       data(i).ibeamstop=float(fields(8))
       data(i).dummy1=float(fields(9))
       data(i).dummy2=float(fields(10))
       data(i).dummy3=float(fields(11))
         end
close,unit
free lun,unit
return, data
end
;-----
function read data,filename
a=read tiff(filename)
a=rebin(a,1024,1024)
return,a
end
;-----
function get beamcenter
print, select points on circle (at least 3 points, end with hitting key)
cursor,x,y,/up,/device
    plots,x-5,y,/device
    plots,x+5,y,/device,color=234,/continue
```

plots,x,y-5,/device

```
plots,x,y+5,/device,color=234,/continue
CX=X
cy=y
i=0
repeat begin
    cursor,x,y,/up,/device
    cx = [cx, x]
    cy=[cy,y]
   plots,x-5,y,/device
    plots,x+5,y,/device,color=234,/continue
    plots,x,y-5,/device
    plots,x,y+5,/device,color=234,/continue
    j=j+1
    end until read key(0) ne 0
return, lsqcirclefit(cx,cy)
end
:-----
function radial_cut,data,phi,npoints,x0,y0
              ; distance sample detector (mm)
d=12700
psize=2*79.1e-3 ;(rebinned) pixel size (mm)
lambda=0.14
                 ; wavelength (nm)
intensity=fltarr(npoints,2)
s phi=sin(0.0174532*phi)
c phi=cos(0.0174532*phi)
for i=0, npoints-1 do begin
         x=fix(x0+i*c phi)
         y=fix(y0+i*s_phi)
         wset,1
         plots,x,y,color=234,/device,/continue
         intensity(i,1)=(data(x,y)+data(x+1,y)+data(x,y+1)+data(x+1,y+1)+data(x-
1,y)+data(x,y-1)+data(x-1,y-1))/7.0
         intensity(i,0)=atan(i*psize/d)/lambda
            end
return, intensity
end
;-----
function collect radial cuts, data, phimin, phimax, phiinc, npoints, x0, y0
radial_cuts=fltarr(npoints,fix(abs(phimin-phimax)/phiinc)+2)
for i=0, n_elements(radial_cuts(0,*))-2 do begin
                 single cut=radial cut(data,phimin+i*phiinc,npoints,x0,y0)
                 radial_cuts(*,i+1)=single_cut(*,1)
                 radial_cuts(*,0)=single_cut(*,0)
                        end
return, radial cuts
end
;-----
function extract base, radial cuts
radial_cuts2=radial_cuts(*,1:n_elements(radial_cuts(0,*))-1)
base=min(radial cuts2,dimension=2)
base=smooth(base,10,/edge truncate)
return.base
end
;-----
function generate 2dbase,base,x0,y0
a=fltarr(1024,1024)
```

for ix=0, 1023 do begin

```
for iy=0, 1023 do begin
           ir=fix(sqrt((ix-x0)*(ix-x0)+(iy-y0)*(iy-y0)))
           if ir lt n elements(base)-2 then a(ix,iy)=(base(ir)+base(ir+1))/2.0
           end
          end
return,a
end
;-----
function f
cursor,x,y,/up,/device
mx=x
my=y
plots,x-5,y,/device
plots,x+5,y,/device,color=234,/continue
plots,x,y-5,/device
plots,x,y+5,/device,color=234,/continue
m=0
    repeat begin
    cursor,x,y,/up,/device
    mx = [mx, x]
    my=[my,y]
    plots,x-5,y,/device
    plots,x+5,y,/device,color=234,/continue
    plots.x.y-5./device
    plots,x,y+5,/device,color=234,/continue
    m=m+1
    end until read key(0) ne 0
return, my
end
·-----
·_____
;Single Plot in 1 Pattern
     _____
:-----
pro test1
window,1,xsize=1024,ysize=1024, title='Show 2D Pattern'
window,2,xsize=1024,ysize=1024, title='Show Plot'
wset.1
data=read_data('test.tif')
tvscl,alog10(data+1)
center=get_beamcenter()
intensity=radial cut(data,45,450,center(0),center(1))
wset,2
plot, intensity (*,0), alog 10 (intensity (*,1)+1)
end
;Multiple plot in 1 Pattern
:-----
              -----
pro test2
loadct.0
window,1,xsize=1024,ysize=1024, title='Show 2D Pattern'
window,2,xsize=1024,ysize=1024, title='Show Plot'
window,3,xsize=1024,ysize=1024, title='Show 2D Background'
window,4,xsize=1024,ysize=1024, title='Show 2D Extracted Data'
wset.1
data=read data('test.tif')
tvscl.alog10(data+1)
center=get beamcenter()
```

radial cuts=collect radial cuts(data,-110,200,1,450,center(0),center(1)) wset,2 plot, radial cuts(*,0), alog10(1+radial cuts(*,1)) for i=0, n_elements(radial_cuts(0,*))-3 do begin oplot,radial_cuts(*,0),alog10(1+radial_cuts(*,i+2)) end base=extract_base(radial_cuts) oplot,radial_cuts(*,0),alog10(base+1),thick=3,color=100 wset,3 background=generate_2dbase(base,center(0),center(1)) tvscl,alog10(background+1) difference=data-background minimum=min(difference) difference(where(difference It 0.0))=0.0 difference=difference-minimum wset.4 tvscl,alog10(difference+1) print, 'min(difference):',min(difference),', ',' max(difference):',max(difference) ;f,difference end ;Data Plot in Different Angles (multiPattern) ;----pro test3,name data=load index(name+'.idx') idx=sort(data.pos) ;plot,data(idx).pos,data(idx).ibeamstop/data(idx).ioni1 plot,data(idx).pos,data(idx).ioni1 end ;Sort and Call Data (multiPattern) ;----pro test4,name window,xsize=1024,ysize=1024 data=load_index(name+'.idx') idx=sort(data.pos) for i=0,n_elements(data)-1 do begin a=read_tiff(data(idx(i)).name) ;i0=data(i).ioni2 ;a=a/i0 ;a=rebin(a,512,512) a=alog10(a+1);tvscl,a ;xyouts,200,50,string(data(i).pos),charsize=3.0,/device if data(idx(i)).ioni1 gt 3000000 then begin print,string(data(idx(i)).pos) a=rebin(a,1024,1024) $a = a \log 10(a+1)$ tvscl,a end end end

:Test5

pro test5,name data=load index(name+'.idx')

idx=sort(data.pos)
for i=0, n_elements(a)-1 do print,a(idx(i)).pos,' ',a(idx(i)).name,' ',a(idx(i)).idoris
end

;Test6

pro test6,indexfile.angle data=load_index(indexfile+'.idx') print,where(data.pos gt angle) print,data(where(data.pos gt angle)).name end ;Isotropic Background Substraction of multiPattern pro test7,name loadct.0 data=load index(name+'.idx') idx=sort(data.pos) ;integral= fltarr(n_elements(data),2) print,'how many data to process?' nd=0 read,nd if nd eq 0 then nd=n elements(data) integral=fltarr(nd,2) window,1.xsize=1024,ysize=1024, title='Show 2D Pattern' wset.1 a=read tiff(data(idx(0)).name) b=rebin(a,1024,1024) $c = a \log 10(b+1)$ tvscl.c center=get beamcenter() for i=0, nd-1 do begin ;n elements(data)-1 do begin wset,1 a=read tiff(data(idx(i)).name) print, string('File:', data(idx(i)).name,', ','loni1:', data(idx(i)).ioni1,', ','Angle:',data(idx(i)).pos) ;if data(idx(i)).ioni1 It 1e7 then begin ;print,' Sorry!, Unwanted' :end if data(idx(i)).ioni1 gt 4*1e6 then begin print, string(data(idx(i)).pos,', ','OK!, Waiting for analysis') a=rebin(a,1024,1024) i0=data(i).ioni2 b=a/i0 ;normalization c=alog10(b+1)tvscl.c xyouts.200.50,string(data(idx(i)).pos),charsize=3.0,/device radial cuts=collect radial cuts(b,-110,200,1,400,center(0),center(1)) window,2,xsize=1024,ysize=1024, title='Show Plot' wset.2 plot,radial cuts(*,0),alog10(1+radial cuts(*,1)) for j=0, n_elements(radial_cuts(0,*))-3 do begin oplot, radial cuts(*,0), alog10(1+radial cuts(*, j+2)) end base=extract base(radial cuts) oplot,radial cuts(*,0),alog10(base+1),thick=3,color=100 window.3,xsize=1024,ysize=1024, title='Show Baseline' wset,3

```
openw, unit, string(data(idx(i)).name,' bas.dat'), /get lun
               base=extract base(radial cuts)
               plot,radial cuts(*,0),alog10(base+1)
               xyouts,200,170, string('Filename:',data(idx(i)).name),charsize=2.0,/device
               xyouts,200,120, string('loni1:',data(idx(i)).ioni1,',
','Angle:',data(idx(i)).pos),charsize=2.0,/device
               xyouts,200,70, string('Max Y:',max(base),', ','Min
Y:',min(base)),charsize=2.0,/device
               printf, unit, string('Filename:',data(idx(i)).name)
               printf, unit, string('Idoris:',data(idx(i)).idoris)
               printf, unit, string('loni1:',data(idx(i)).ioni1)
               printf, unit, string('Ioni2:',data(idx(i)).ioni2)
               printf, unit, string('lbeamstop:',data(idx(i)).ibeamstop)
               printf, unit, string('Angle:',data(idx(i)).pos)
               printf, unit, string('Accutime:',data(idx(i)).accutime)
               printf, unit, string('Max Y:',max(base),', ','Min Y:',min(base))
                  for k=0, n elements(base)-1 do begin
                  printf, unit, radial_cuts(k,0), base(k)
                  end
               close, unit
               free lun, unit
               ;window,4,xsize=1024,ysize=1024, title='Show 2D Background'
               :wset.4
               background=generate 2dbase(base,center(0),center(1))
               ;tvscl,alog10(background+1)
               difference=b-background
               minimum=min(difference)
               difference(where(difference lt 0.0))=0.0
               difference=difference-minimum
               ;window,5,xsize=1024,ysize=1024, title='Show 2D Extracted Data'
               ;wset,5
               ;tvscl,alog10(difference+1)
               print, 'min(difference):',min(difference),',
                                                            ',' max(difference):',max(difference)
         ;Analysis
            x=double(radial cuts(*,0))
            ff=double(base)
            curve area = int tabulated( x, ff, /double, /sort)
            print, string('Curve Area of', data(idx(i)).name, '=', curve_area)
            integral(i,0)= data(idx(i)).pos
            integral(i,1) = curve area
        end
       end
window,6, title='Plot of Integral'
wset.6
plot, integral(*,0), integral(*,1)
openw,unit,string(name,'_','integralcurve.txt'), /get_lun
    for p=0, nd-1 do begin
    printf, unit, integral(p,0), integral(p,1)
    end
close.unit
free lun.unit
end
```