Diamond Uses of DAWN Science

NOBUGS 2014

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Content

1. Introduction to DAWN Science
2. Java interfaces for data analysis and visualization
3. Applications at Diamond
4. Future developments

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Data Analysis WorkbeNch

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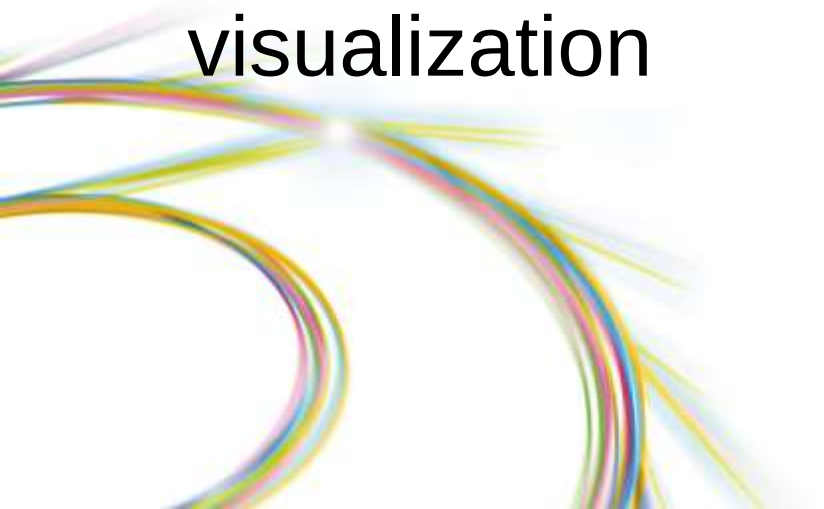
- Eclipse plugin technology based on OSGi
- Science Working Group for interoperability of plugins
- Incubator project
- Definition of interfaces and services necessary for data analysis and visualization



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Data access

- Loader service for many file formats:
  - HDF5
  - CBF
  - common images PNG, TIFF, etc
  - proprietary area detector outputs
  - plugin extendibility for other formats

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Datasets

- N-dimensional, multiple types
- Lazy loading capability
- Slicing for subsets
- NumPy-like broadcasting in many operations
- Library of mathematical and statistical operations

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Metadata

- Can be loaded independently of data
- Associated with files and also datasets
- Experimental context and environment
- Units, errors, scan positions, etc

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Data visualization

- Standard line and image plots provided by Eclipse Nebula project's XY graph
- 2D surface plots with jReality

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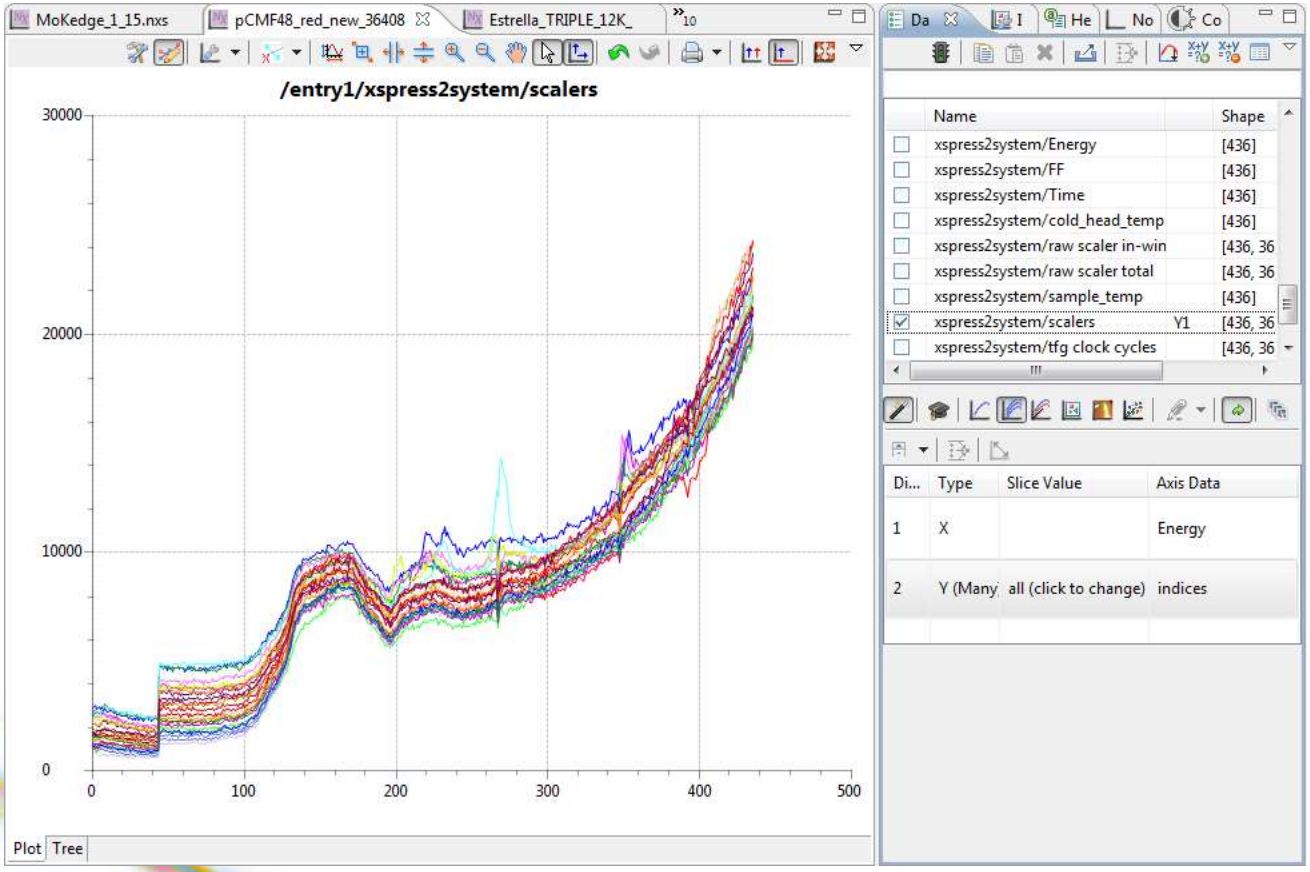
MoKedge_1_15.nxs
pCMF48_red_new_36408
Estrella_TRIPLE_12K_
/entry1/xspress2system/scalers
30000
20000
10000
0
0
100
200
300
400
500
Plot
Tree
Name
Shape
xspress2system/Energy [436]
xspress2system/FF [436]
xspress2system/Time [436]
xspress2system/cold_head_temp [436]
xspress2system/raw scaler in-win [436, 36
xspress2system/raw scaler total [436, 36
xspress2system/sample_temp [436]
xspress2system/scalers Y1 [436, 36
xspress2system/tfg clock cycles [436, 36
Di...
Type
Slice Value
Axis Data
1 X Energy
2 Y (Many all (click to change) indices

Data visualization

- Standard line and image plots provided by Eclipse Nebula project's XY graph
- 2D surface plots with jReality

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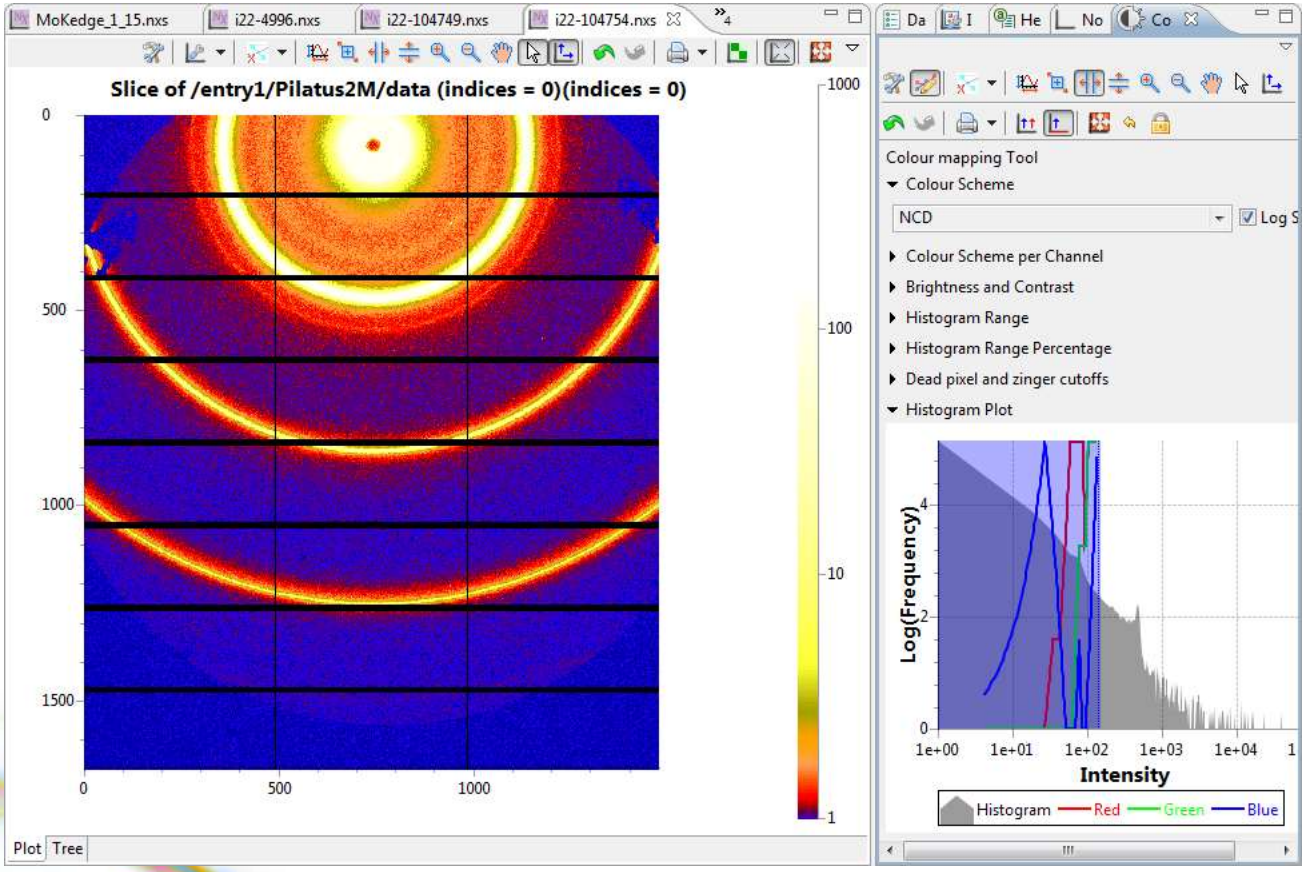
MoKedge_1_15.nxs
i22-4996.nxs
i22-104749.nxs
i22-104754.nxs
Slice of /entry1/Pilatus2M/data (indices = 0)(indices = 0)
0
500
1000
1500
0
500
1000
1000
100
10
1
Plot
Tree
Da
I
He
No
Co
Colour mapping Tool
Colour Scheme
NCD
Log S
Colour Scheme per Channel
Brightness and Contrast
Histogram Range
Histogram Range Percentage
Dead pixel and zinger cutoffs
Histogram Plot
Log(Frequency)
4
2
0
1e+00
1e+01
1e+02
1e+03
1e+04
Intensity
Histogram
Red
Green
Blue

Data visualization

- Standard line and image plots provided by Eclipse Nebula project's XY graph
- 2D surface plots with jReality

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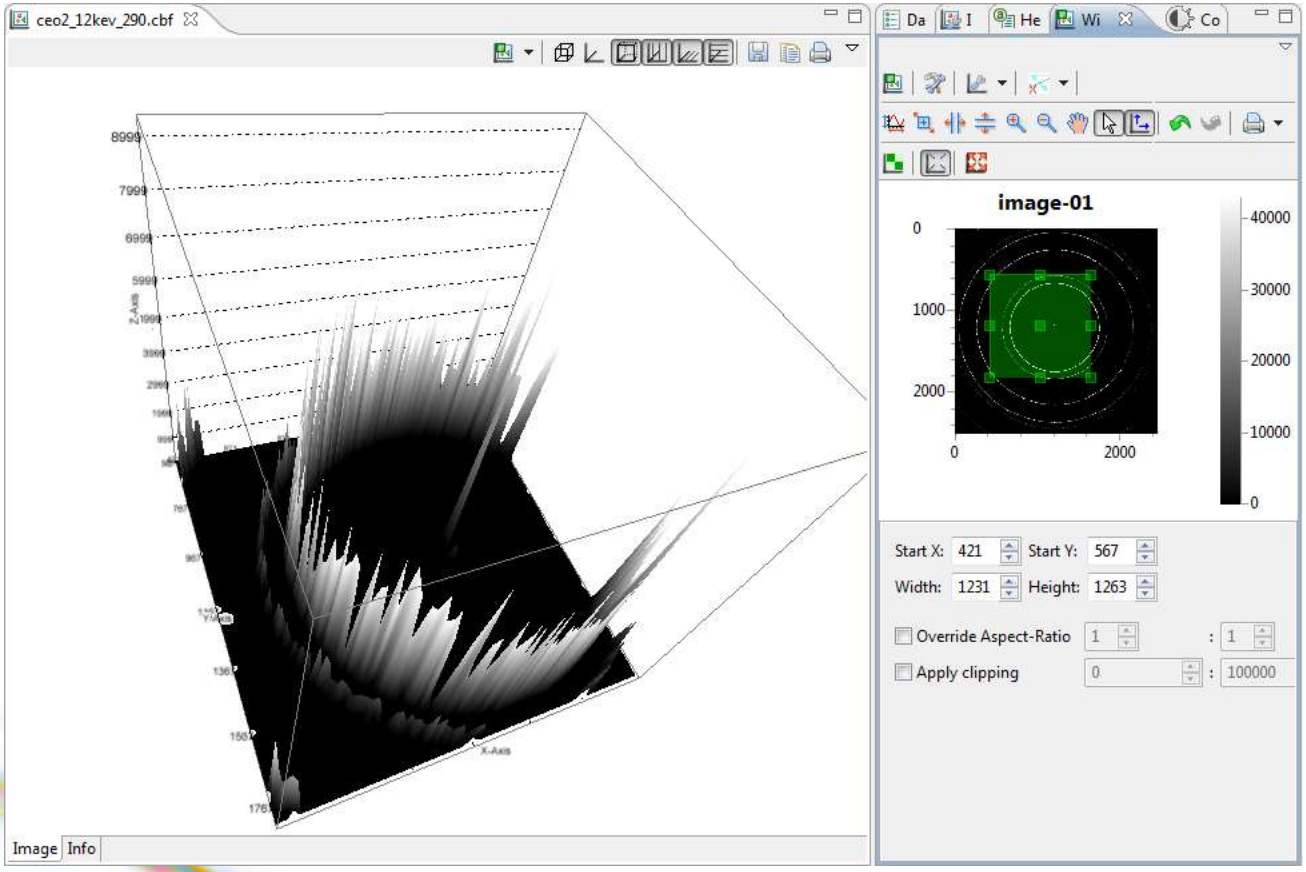
ceo2_12kev_290.cbf
Da
I
He
Wi
Co
8999
7999
6999
5999
Z-Axis
X-Axis
Image
Info
image-01
0
1000
2000
0
2000
40000
30000
20000
10000
0
Start X: 421
Start Y: 567
Width: 1231
Height: 1263
Override Aspect-Ratio
Apply clipping

Regions of Interest

- Many 0D, 1D and 2D regions provided:
  - Point, line, polyline, conic sections
  - Polygon, ellipse, annular sector
- GUI tools for interactive creation with displayed data

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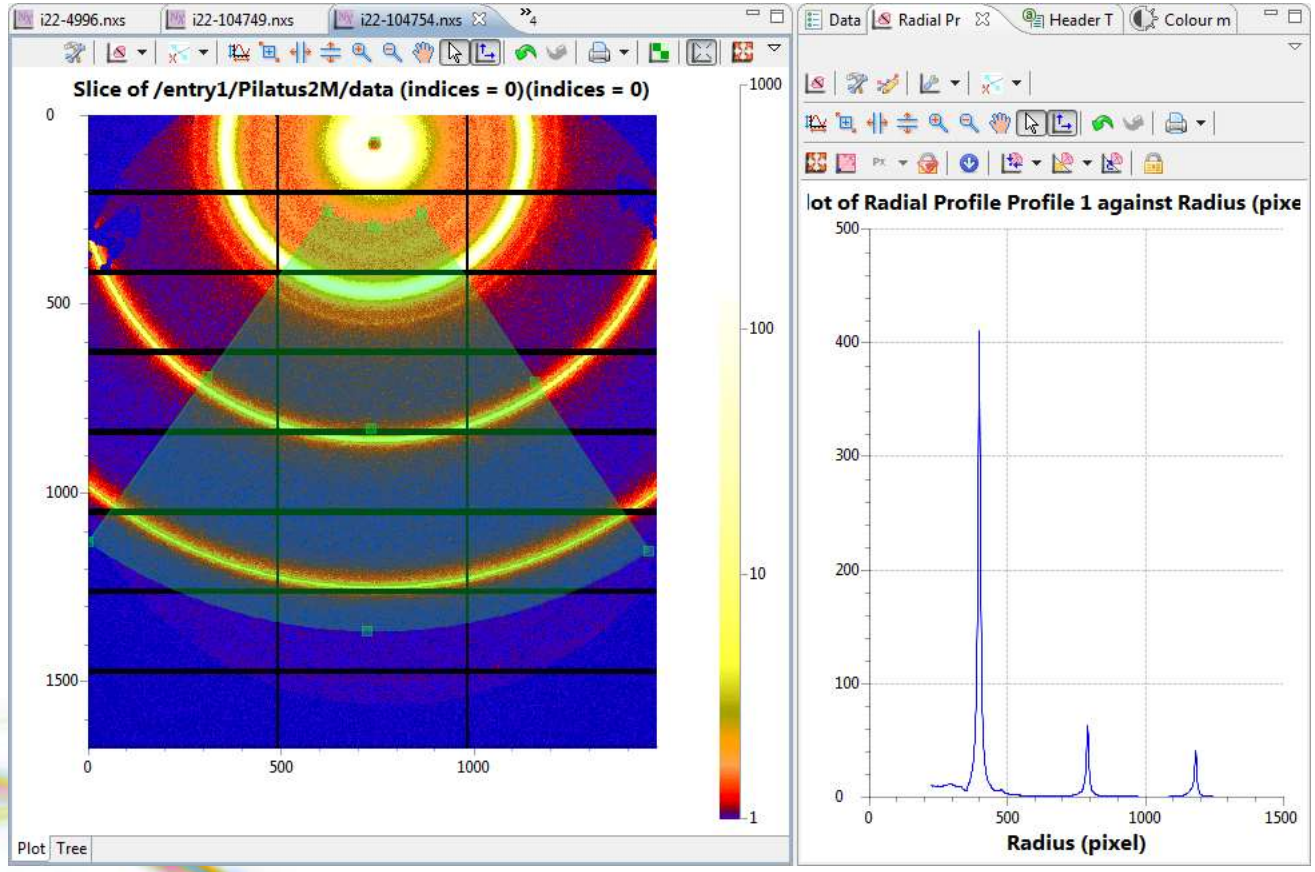
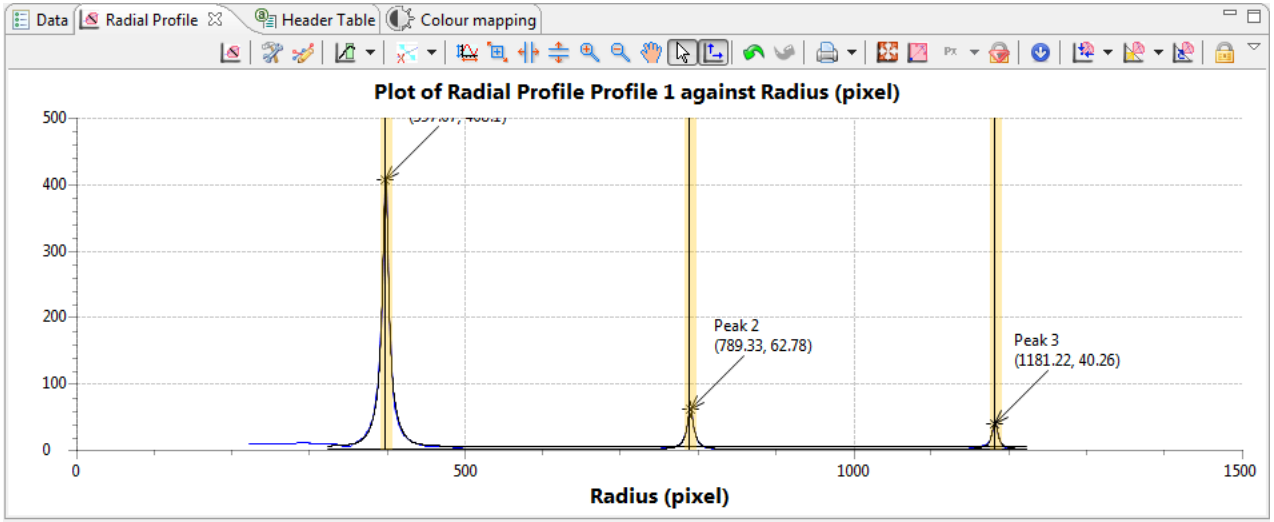
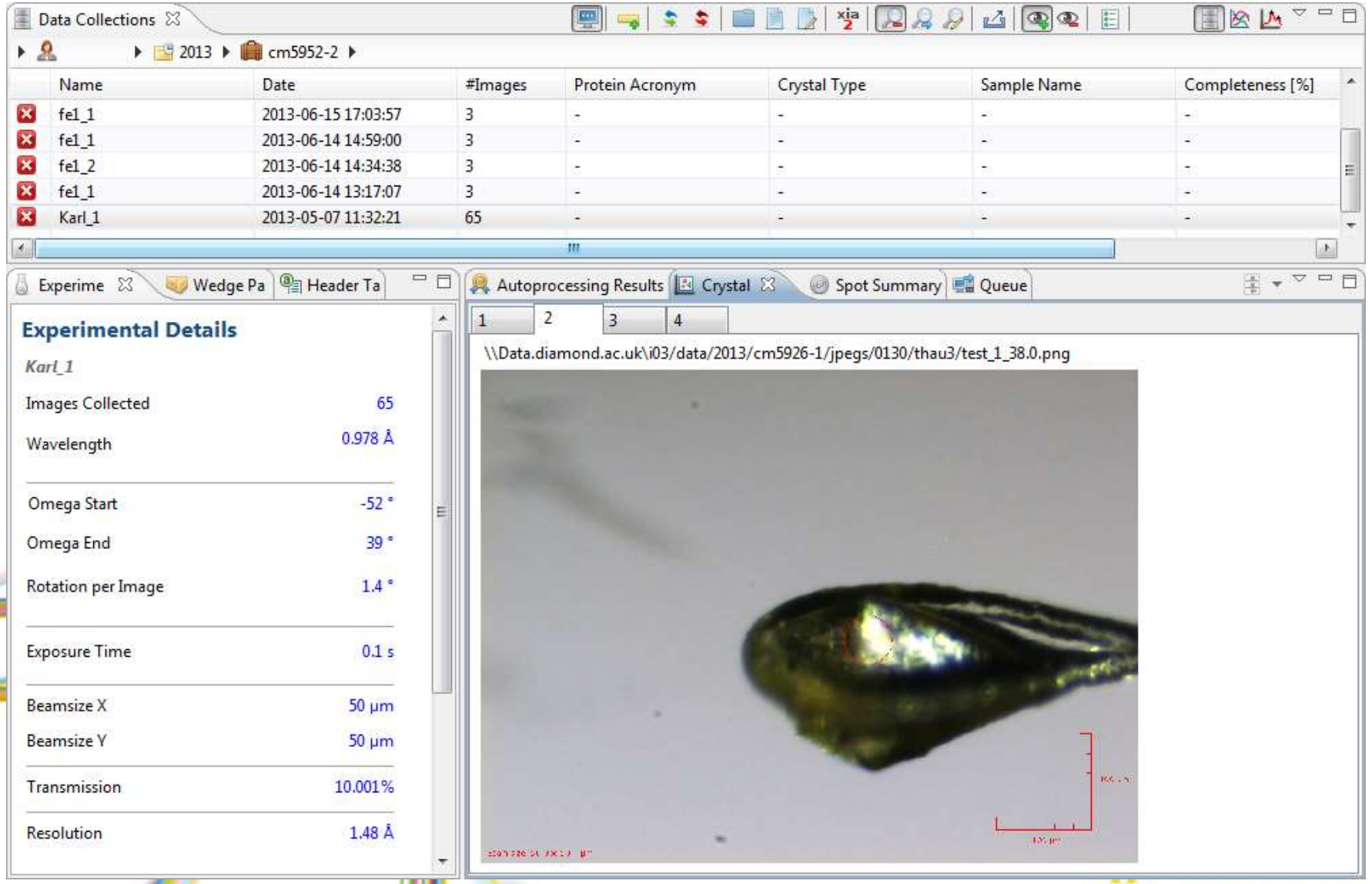

i22-4996.nxs
i22-104749.nxs
i22-104754.nxs
Slice of /entry1/Pilatus2M/data (indices = 0)(indices = 0)
0
500
1000
1500
0
500
1000
1000
100
10
1
Plot
Tree
Data
Radial Pr
Header T
Colour m
lot of Radial Profile Profile 1 against Radius (pixe
500
400
300
200
100
0
0
500
1000
1500
Radius (pixel)

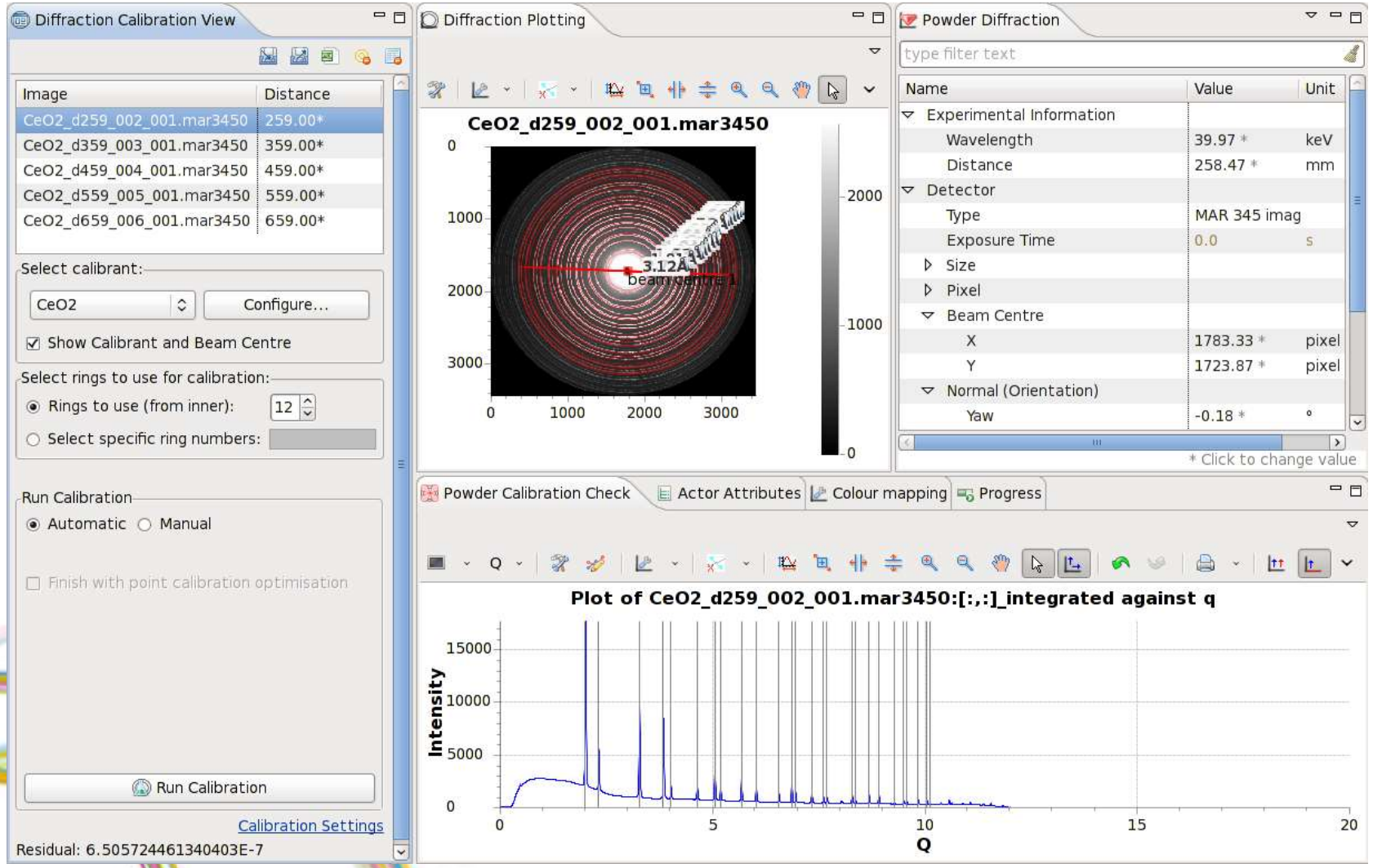

Data
Radial Profile
Header Table
Colour mapping
Plot of Radial Profile Profile 1 against Radius (pixel)
500
400
300
200
100
0
0
500
1000
1500
Peak 2
(789.33, 62.78)
Peak 3
(1181.22, 40.26)
Radius (pixel)
Peak Fitting
Trace
Name
Position
Fit
FWHM
Area
Type
Algorithm
Radial Profi...
Peak 1
397.0682
408.10154
10.01174
6456.74882
PseudoVoigt
GeneticAlg
Radial Profi...
Peak 2
789.33258
62.77947
10.04722
986.68122
PseudoVoigt
GeneticAlg
Radial Profi...
Peak 3
1181.22496
40.2571
10.16054
722.66829
PseudoVoigt
GeneticAlg
Fit attempted: '3' PseudoVoigt's using GeneticAlg with smoothing of '1' (configure smoothing)

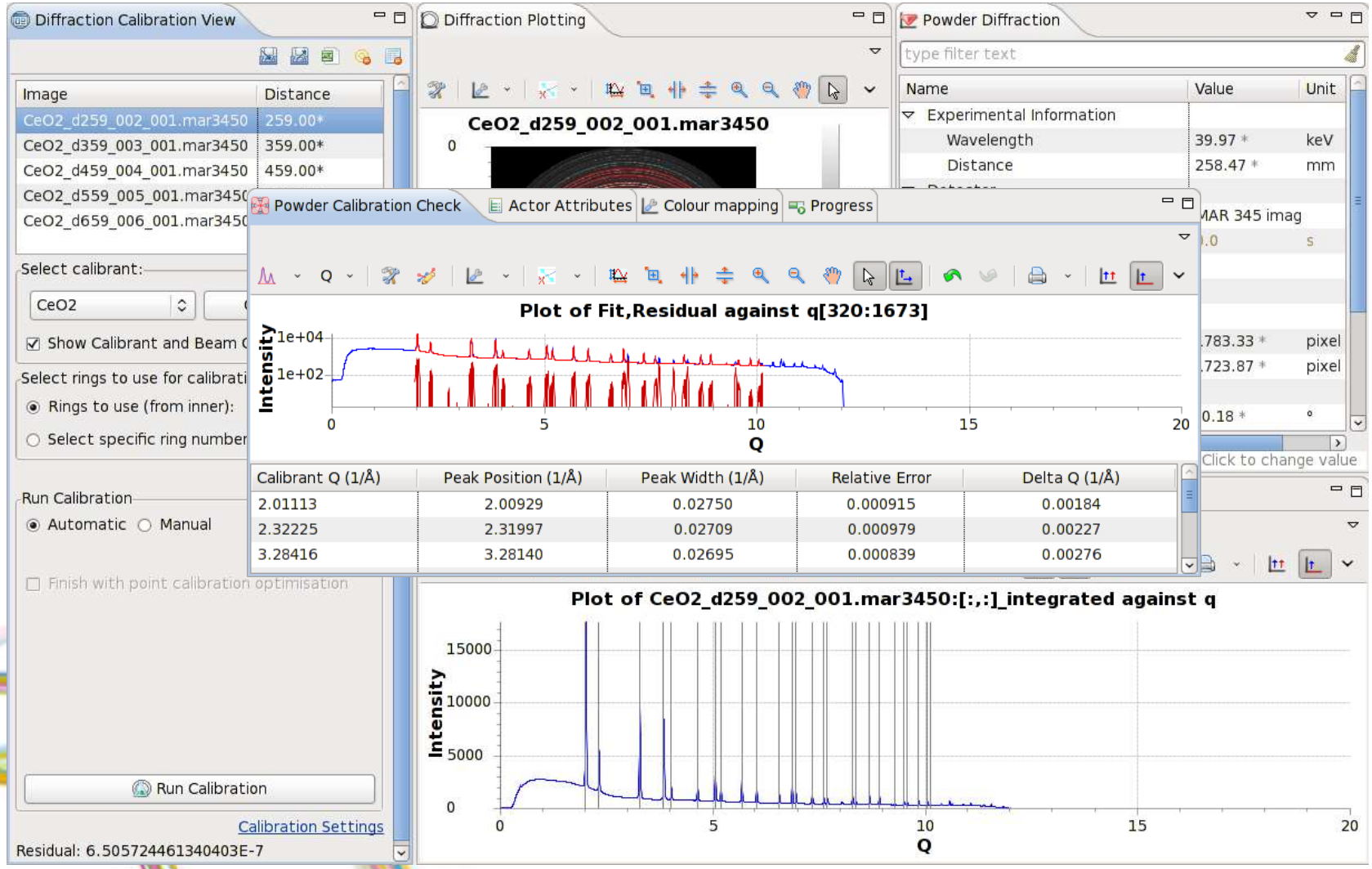
ISPyB explorer

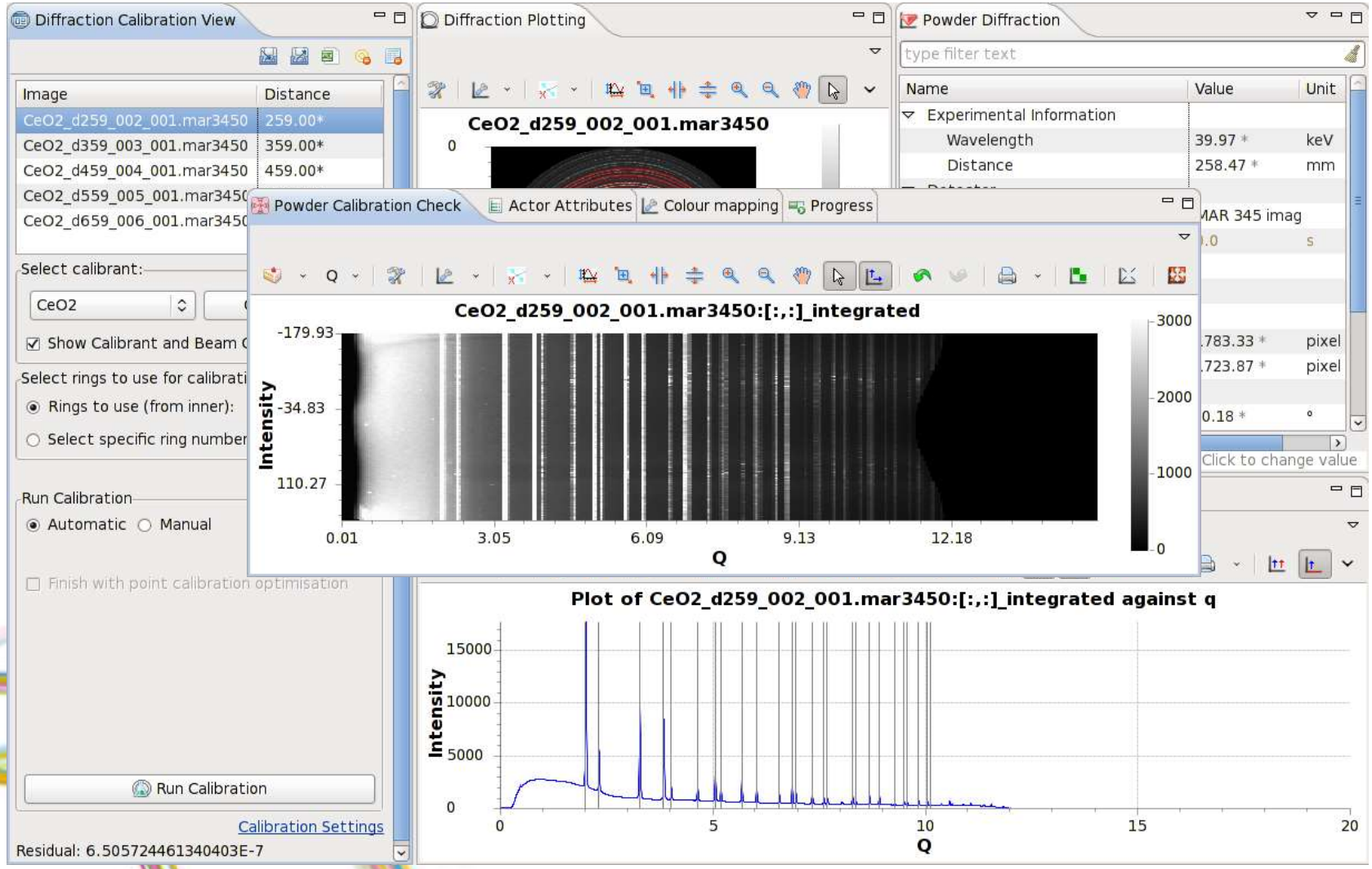


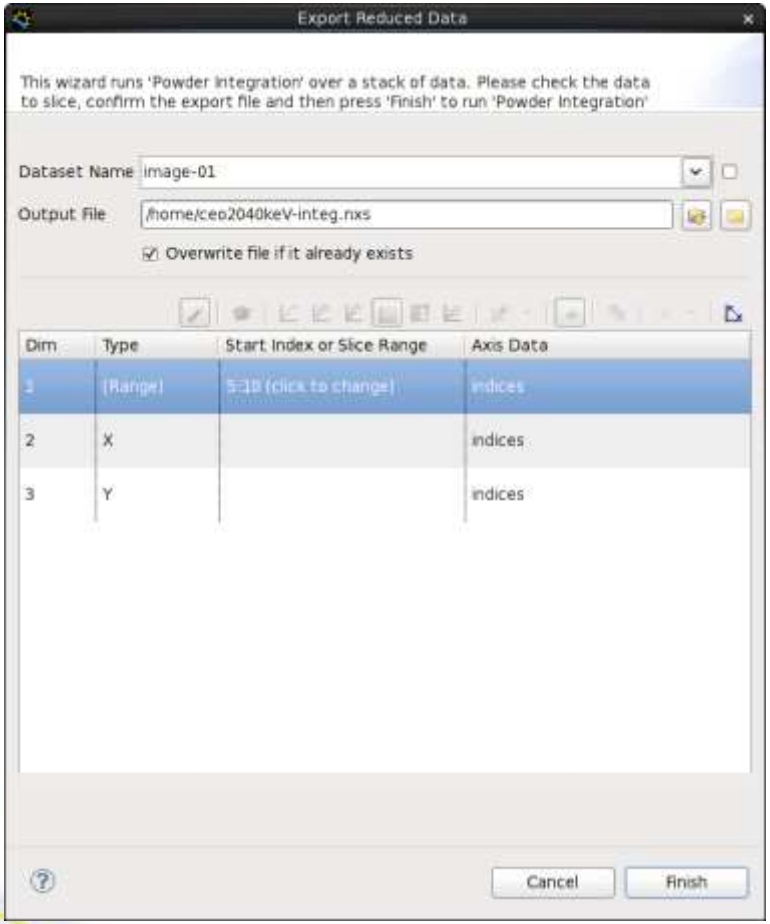
2D powder diffraction

- Calibrate detector orientation and position and source wavelength with images of calibrant diffraction rings
- Reduce multiple images of test material


Diffraction Calibration View
Image
Distance
CeO2_d259_002_001.mar3450
259.00*
CeO2_d359_003_001.mar3450
359.00*
CeO2_d459_004_001.mar3450
459.00*
CeO2_d559_005_001.mar3450
559.00*
CeO2_d659_006_001.mar3450
659.00*
Select calibrant:
CeO2
Configure...
Show Calibrant and Beam Centre
Select rings to use for calibration:
Rings to use (from inner):
12
Select specific ring numbers:
Run Calibration
Automatic
Manual
Finish with point calibration optimisation
Run Calibration
Calibration Settings
Residual: 6.505724461340403E-7
Diffraction Plotting
CeO2_d259_002_001.mar3450
3.12Å
Beam Centre: 1
Powder Diffraction
type filter text
Name
Value
Unit
Experimental Information
Wavelength
39.97 *
keV
Distance
258.47 *
mm
Detector
Type
MAR 345 imag
Exposure Time
0.0
s
Size
Pixel
Beam Centre
X
1783.33 *
pixel
Y
1723.87 *
pixel
Normal (Orientation)
Yaw
-0.18 *
°
* Click to change value
Powder Calibration Check
Actor Attributes
Colour mapping
Progress
Plot of CeO2_d259_002_001.mar3450:[:,:]_integrated against q
Intensity
Q

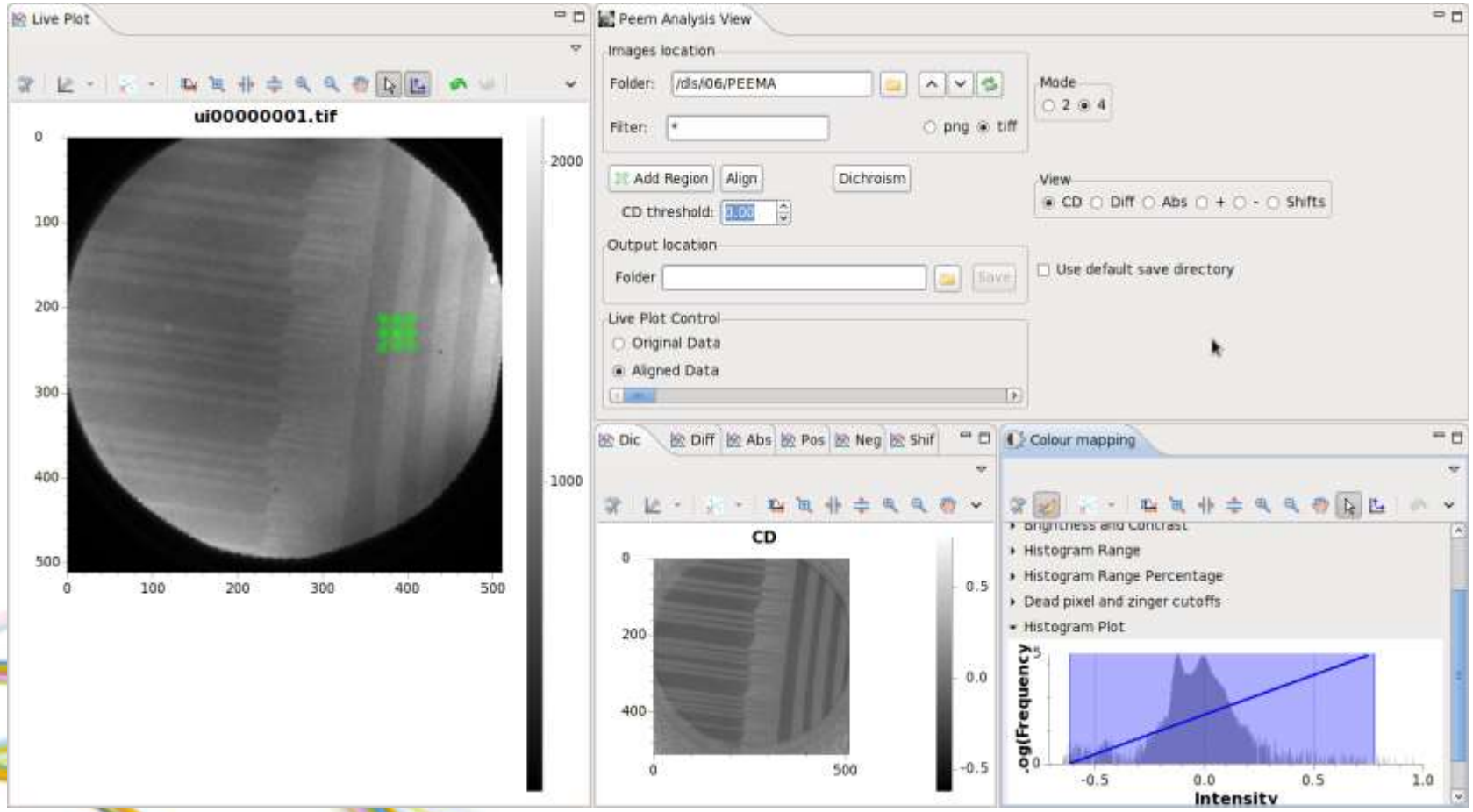

Diffraction Calibration View
Image
Distance
CeO2_d259_002_001.mar3450
259.00*
CeO2_d359_003_001.mar3450
359.00*
CeO2_d459_004_001.mar3450
459.00*
CeO2_d559_005_001.mar3450
CeO2_d659_006_001.mar3450
Select calibrant:
CeO2
Show Calibrant and Beam
Select rings to use for calibrati
Rings to use (from inner):
Select specific ring number
Run Calibration
Automatic
Manual
Finish with point calibration optimisation
Run Calibration
Calibration Settings
Residual: 6.505724461340403E-7
Diffraction Plotting
CeO2_d259_002_001.mar3450
Powder Diffraction
type filter text
Name
Value
Unit
Experimental Information
Wavelength
39.97 *
keV
Distance
258.47 *
mm
MAR 345 imag
.783.33 *
pixel
.723.87 *
pixel
0.18 *
Click to change value
Powder Calibration Check
Actor Attributes
Colour mapping
Progress
Plot of Fit,Residual against q[320:1673]
Intensity
1e+04
1e+02
Q
Calibrant Q (1/Å)
Peak Position (1/Å)
Peak Width (1/Å)
Relative Error
Delta Q (1/Å)
2.01113
2.00929
0.02750
0.000915
0.00184
2.32225
2.31997
0.02709
0.000979
0.00227
3.28416
3.28140
0.02695
0.000839
0.00276
Plot of CeO2_d259_002_001.mar3450:[:,:]_integrated against q
Intensity
Q


Diffraction Calibration View
Image
Distance
CeO2_d259_002_001.mar3450
259.00*
CeO2_d359_003_001.mar3450
359.00*
CeO2_d459_004_001.mar3450
459.00*
CeO2_d559_005_001.mar3450
CeO2_d659_006_001.mar3450
Select calibrant:
CeO2
Show Calibrant and Beam
Select rings to use for calibrati
Rings to use (from inner):
Select specific ring number
Run Calibration
Automatic
Manual
Finish with point calibration optimisation
Run Calibration
Calibration Settings
Residual: 6.505724461340403E-7
Diffraction Plotting
CeO2_d259_002_001.mar3450
Powder Diffraction
type filter text
Name
Value
Unit
Experimental Information
Wavelength
39.97 *
keV
Distance
258.47 *
mm
MAR 345 imag
.783.33 *
pixel
.723.87 *
pixel
0.18 *
Click to change value
Powder Calibration Check
Actor Attributes
Colour mapping
Progress
Q
CeO2_d259_002_001.mar3450:[:,:]_integrated
-179.93
-34.83
110.27
Intensity
0.01
3.05
6.09
9.13
12.18
Q
3000
2000
1000
0
Plot of CeO2_d259_002_001.mar3450:[:,:]_integrated against q
15000
10000
5000
0
Intensity
0
5
10
15
20
Q


Export Reduced Data
This wizard runs 'Powder Integration' over a stack of data. Please check the data to slice, confirm the export file and then press 'Finish' to run 'Powder Integration'
Dataset Name
image-01
Output File
/home/ceo2040keV-integ.nxs
Overwrite file if it already exists
Dim
Type
Start Index or Slice Range
Axis Data
1
[Range]
5:10 (click to change)
indices
2
X
indices
3
Y
indices
Cancel
Finish

Photoelectron emission microscopy – XMCD analysis

- Inspect and align images
- Calculate circular dichroism


Live Plot
ui00000001.tif
Peem Analysis View
Images location
Folder:
/dls/i06/PEEMA
Filter:
*
png
tiff
Mode
2
4
Add Region
Align
Dichroism
CD threshold:
1.00
View
CD
Diff
Abs
+
-
Shifts
Output location
Folder
Save
Use default save directory
Live Plot Control
Original Data
Aligned Data
Dic
Diff
Abs
Pos
Neg
Shif
CD
Colour mapping
Histogram Range
Histogram Range Percentage
Dead pixel and zinger cutoffs
Histogram Plot
Intensity

Future work

- Commit concrete implementations to Eclipse project
- More visualization including volume rendering of isosurfaces with JavaFX
- Lazy or deferred evaluation of operations on datasets
- Error propagation in operations on datasets

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- For more details on the applications shown and other DAWN applications (including angle-resolved photoelectron emission spectroscopy data reduction), see posters PS-01 and PS-16
- Check out www.dawnsci.org