

The short guide

DIAMOND ANVIL CELL

Calibration with LaB6:

Conversion of images with marcvt:

- marcvt -tiff16 Lab6_003.mar3450
- marcvt -tiff16 MgFeO_25keV_006.mar3450

New analysis

Instrument: ALS_12.2.2

- Angular calibration -> Inclined (Reflection) Image: Detector distance: 350
- Geometry -> Image 2D
- Measurement -> 2Theta
- Source -> Synchrotron: Wavelength: 0.49594
- Instrument Broadening -> Caglioti PV:
 - Asymmetry: 0
 - HWHM: 0.0025 0 0

Datafiles:

From Images...: Load: Lab6_001.tiff16

- Adjust brightness/contrast, set 0-100
- Oval selection
- Plugins->Multi spectra from flat reflection image
 - Center X: 173
 - Center Y: 154.9
 - Eta step: 5 degs or 10 degs
 - uncheck 2Theta angles calibrates and reflection image

Background: (v1) - 12 polynomial background pars, Chebychev

(V2) - remove common polynomial, add 5 parameters for all datafiles

Range: 6-28

Add to phases: LAB6.cif

- Cell: 4.15689
- Size/strains: 7000 / 1E-5

Compute pattern

Add excluded regions: 8-9, 12.5-14.6, 17.2-18, 24-25.5

Add bkg peak: 10, 20.7, 0.1

Refine:

- Background, scale parameters, image centering, tilting, detector distance, bound B factors
- All Caglioti, All B factors

- Arbitrary texture fix B factors

Save analysis, fix all parameters, export instrument in instrument.mdb

RDAC WITH MG0.9FE0.1O

New analysis

Import instrument ALS_12.2.2

Datafiles:

Drag and drop: MgFeO_25KeV_003.tiff16

Range: 10.7-24.5

Check plot, remove 51-52 patterns

Add phase MgFeO.cif

- Occupation Mg 0.9, Fe 0.1
- Select EWIMV, 7.5 cell, cylindrical symmetry
- Select Moment Pole Stress: C11: 578.25, C12:161.9, C44:76
S11=S22, S33 = -2*S11, use texture, BulkPathGEO model

Compute pattern, adjust bkg, cell par

Adjust S11 with 2D plot

Refine: scale factors, bound B factor, image centering, cell, microstructure, S11

Add background interpolated: 20 points

Refine O occupancy

Save analysis and check results