High-pressure single-crystal x-ray diffraction data processing with XDS

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The following manual is based on our experience with the data collected at the beamline D3 at HASYLAB (a four-circle HUBER diffractometer with a marCCD165 detector). However, all the important procedures and tricks described here are general. For the "hardware", distortion, noise, detector position, and incident beam parameters, etc., that are specific to other detectors (formats) and facilities, see the XDS templates. The correctness of the manual has now been tested with the data measured on the beamline P02 at Petra-III (an ω axis and a mar345 detector).

X-ray **D**iffraction **S**oftware: XDS, XSCALE, XDSCONV

W. Kabsch, *J. Appl. Cryst*. **21**, 916 (1988)

W. Kabsch, *Acta Cryst*. D**66**, 125-132 (2010)

W. Kabsch, *Acta Cryst*. D**66**, 133-144 (2010)

http://xds.mpimf-heidelberg.mpg.de

Originally written for biological crystallography that most of the times deals with bad data due to ice rings, radiation damages, metastable phases, coexisting phases, poorly crystalline materials, etc. Bad data is exactly what a high-pressure crystallographer has to work with.

XDS: data indexing, integration, and correction for area-sensitive detectors

XSCALE: combining the data from different runs and correcting them for absorption and radiation damage

XDSCONV: hkl data conversion to different formats

XDS.INP file templates for various detectors

http://xds.mpimf-heidelberg.mpg.de/html_doc/xds_prepare.html

file name	detector
XDS-PILATUS.INP	PILATUS 6M pixel detector designed at PSI/SLS (Broennimann et al.)
XDS-ADSC.INP	ADSC detectors Quantum Q4, Q4r, Q105, Q210, Q210r, Q315r & Q315
XDS-NOIR.INP	Ed Westbrook's NOIR-1 lens focused CCD detector at ALS 4.2.2
XDS-MAR555.INP	Selenium based flat panel detector
XDS-MAR345.INP	MAR345 detector
XDS-MAR.INP	old MAR-detector
XDS-MARCCD.INP	MAR CCD-detector and (1k X 1k)-CCD used at CHESS
XDS-RAXIS2.INP	R-AXIS II IMAGING PLATE DETECTOR
XDS-RAXIS4.INP	R-AXIS IV IMAGING PLATE DETECTOR
XDS-RAXIS4++.INP	R-AXIS IV++ IMAGING PLATE DETECTOR
XDS-RAXIS5.INP	R-AXIS V IMAGING PLATE DETECTOR
XDS-SATURN.INP	Rigaku/MSC CCD detector
XDS-CRYSALIS.INP	Oxford Diffraction CCD detector
XDS-CCDBRANDEIS.INP	(2080 X 2072)-CCD Detector used at BNL X12c; (1k X 1k)-CCD Detector (Walter Phillips) used at BNL
XDS-BRANDEIS_B4.INP	(2k X 2k)-CCD Detector used at Brookhaven beamline B4
XDS-STOE.INP	STOE IMAGING PLATE DETECTOR
XDS-SIEMENS.INP	X100A SIEMENS Multiwire detector

Features of XDS to consider while working with high-pressure single-crystal x-ray data

Pros:

1. Free software to process the data from several detectors on laboratory diffractometers and at synchrotron facilities.
2. Learned "*Kabsch*" reflection profiles. Recorded spots/reflections on area-sensitive detectors are distorted due to their trajectory in the Ewald sphere. Kabsch devised a transformation from the rotation geometry to a precession-like geometry, in which all the reflections have the same profile.
3. Gasket rings (or any Debye-Scherrer rings) could be treated like ice rings in the standard use of XDS.
4. When used with care, it produces excellent high-pressure *hkl* data.
5. Very easy to use.

Cons:

1. No reciprocal space reconstruction.
2. Does not handle incommensurate phases.
3. Kind of a "black box" with some cryptic actions (especially in CORRECT) – it is too automatic, tends to get wild, and tries to do too much for the "high-pressure" user.
4. Poor graphics and visualization of the data and results when compared to commercial software. However, there are some GUIs to run XDS available on the web, e.g., *J. Appl. Cryst*. **45**, 568-572 (2012).
5. No possibility to exclude shadowed areas of a detector by a diamond anvil cell from the integration process. It has problems to perform integration in the DAC shadows as it just "generates" some non-sense numbers with negative sigmas. A large number of the shaded reflections could be rejected by setting up a proper global background.

1. **XDS: 8 subroutines**

XYCORR performs spatial corrections at each pixel of a detector

INIT classifies pixels as background or strong (diffraction) spots

COLSPOT locates strong diffraction spots and finds their centroids

IDXREF finds and refines the orientation matrix

DEFPIX defines the obscured regions of the detector by intruding hardware, e.g., a cryostat (not useful for masking the shifting shadowed areas of the detector by a diamond anvil cell)

XPLAN supports the planning of data collection (a run optimizer)

INTEGRATE determines the intensities, updates profiles, and refines parameters

CORRECT applies various corrections to the intensities, determines the space group if unknown, and refines the unit-cell parameters

An example of XDS.INP for high-pressure data (marCCD165) from the beamline D3 at HASYLAB

```
!*******************************************************************************
!  Example
!*******************************************************************************


 JOB= XDS
! JOB= COLSPOT IDXREF DEFPIX XPLAN INTEGRATE CORRECT
! JOB= IDXREF DEFPIX XPLAN INTEGRATE CORRECT
! JOB= DEFPIX INTEGRATE CORRECT
! JOB= INTEGRATE CORRECT
! JOB= CORRECT

NAME_TEMPLATE_OF_DATA_FRAMES=../frames/BiMn2O5_P2_05_????.tif                 ! INIT, COLSPOT, IDXREF, INTEGRATE
DATA_RANGE=       1  60  !Numbers of first and last data frame collected      ! COLSPOT, INTEGRATE, CORRECT
BACKGROUND_RANGE= 41 42  !Numbers of first and last data frame for background ! INIT
SPOT_RANGE=       30 40  !First and last data frame number for finding spots  ! COLSPOT, IDXREF

INCLUDE_RESOLUTION_RANGE= 15.0 0.0                                            ! DEFPIX, CORRECT
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS= 4000 30000                           ! DEFPIX

ORGX=1069.4 ORGY=1020.6   !Origin on detector (pixels)                        ! IDXREF

DIRECTION_OF_DETECTOR_X-AXIS=  0 0 1
DIRECTION_OF_DETECTOR_Y-AXIS=  0 1 0
INCIDENT_BEAM_DIRECTION=      -1 0 0
ROTATION_AXIS=  0.086824089 0.866025404 -0.492403877 ! direction cosines with respect to the laboratory system

DETECTOR_DISTANCE=  81.38          !Distance of detector from crystal-mm      ! IDXREF
OSCILLATION_RANGE=   1.0           !Of each data frame in degrees (must be >0) ! IDXREF
STARTING_ANGLE=    238.1           !Of spindle at beginning of data frame #1.  ! IDXREF
X-RAY_WAVELENGTH=    0.4           !X-ray wavelength in Angstroem units

SPACE_GROUP_NUMBER=     1                                                     ! IDXREF, CORRECT
UNIT_CELL_CONSTANTS=    7.5 8.5 5.7 90.0 90.0 90.0                            ! IDXREF, CORRECT
! UNIT_CELL_A-AXIS=
! UNIT_CELL_B-AXIS=
! UNIT_CELL_C-AXIS=

!REIDX= -1 0 0 0  0 1 0 0  0 0 -1 0                                           ! CORRECT
FRIEDEL'S_LAW=FALSE                                                           ! XPLAN, CORRECT
```

```
INDEX_ORIGIN= 0 0 0                                                          ! IDXREF

BEAM_DIVERGENCE=          0.50  !arctan(spot diameter/DETECTOR_DISTANCE)     ! INTEGRATE
BEAM_DIVERGENCE_E.S.D.=   0.05  !half-width (Sigma) of BEAM_DIVERGENCE=      ! INTEGRATE
REFLECTING_RANGE=         0.30  !for crossing the Ewald sphere on shortest route   ! COLSPOT, IDXREF, INTEGRATE
REFLECTING_RANGE_E.S.D.=  0.04  !half-width (mosaicity) of REFLECTING_RANGE=     ! INTEGRATE

DELPHI= 10.0                                                                 ! INTEGRATE

!*****************************************************************************

MAXIMUM_NUMBER_OF_PROCESSORS=  2                                             ! COLSPOT, IDXREF, INTEGRATE, CORRECT
MINUTE=     1    !Maximum number of minutes to wait until data frame must appear ! XYCORR, INIT, COLSPOT, INTEGRATE
TEST=       1    !Test flag. 1, 2 additional diagnostics and images          ! XYCORR, INIT, COLSPOT, INTEGRATE

! Detector description MARCCD 165
DETECTOR=     CCDCHESS                                                       ! XYCORR, INTEGRATE
NX=2048       NY=2048                                                        ! XYCORR, INIT, COLSPOT, IDXREF
QX=0.079076   QY=0.079076                                                    ! XYCORR, IDXREF

OVERLOAD=50000                                                               ! XYCORR, INIT, COLSPOT, INTEGRATE, CORRECT
! MINIMUM_VALID_PIXEL_VALUE= 0                                               ! INIT, COLSPOT, INTEGRATE

TRUSTED_REGION= 0.0 1.0                                                      ! INIT, IDXREF

UNTRUSTED_RECTANGLE= 1010 1110 0 1000                                        ! INIT

! EXCLUDE_RESOLUTION_RANGE= 3.93 3.87 ! ice-ring at 3.897                    ! DEFPIX, CORRECT

FRACTION_OF_POLARIZATION=   0.950   ! 0.5 for unpolarized beam               ! CORRECT
POLARIZATION_PLANE_NORMAL=  0.0 0.0 1.0                                      ! CORRECT

MAX_CELL_AXIS_ERROR=    0.03        ! default = 0.03                         ! IDXREF, CORRECT
MAX_CELL_ANGLE_ERROR=   2.0         ! default = 2.0                          ! IDXREF, CORRECT

TEST_RESOLUTION_RANGE=  10.0  2.0                                            ! CORRECT
MIN_RFL_Rmeas=          25          ! default = 50                           ! CORRECT
MAX_FAC_Rmeas=          2.0                                                  ! CORRECT

! REFINE(IDXREF)=BEAM AXIS ORIENTATION DISTANCE CELL    ! or: ALL           ! IDXREF
! REFINE(INTEGRATE)=BEAM AXIS ORIENTATION DISTANCE CELL ! or: ALL           ! INTEGRATE
! REFINE(CORRECT)=BEAM AXIS ORIENTATION DISTANCE CELL   ! or: ALL           ! CORRECT

WFAC1= 50.0
```

```
STRICT_ABSORPTION_CORRECTION= TRUE     ! default = FALSE                    ! CORRECT

CORRECTIONS=!  ALL MODULATION DECAY ABSORPTION                              ! CORRECT

!REFLECTIONS/CORRECTION_FACTOR= 100   ! default approx. 50                  ! CORRECT
```

Important input parameters in file XDS.INP (apart from the specific "hardware", distortion, noise, detector position, and incident beam parameters for the specific detector and format).

DATA_RANGE – the first and last data image

BACKGROUND_RANGE – the first and last data image to determine the background

SPOT_RANGE – the first and last data image to identify and locate strong spots for indexing

ROTATION_AXIS – direction cosines of the rotation axis with respect to the laboratory system. The direction of the axis is chosen to describe a right-handed rotation.

STARTING_ANGLE – the phi angle of the first data image in SPOT-RANGE

SPACE_GROUP_NUMBER – while using XDS for the high-pressure data it always has to be 1

EXCLUDE_RESOLUTION_RANGE – used for any ice/gasket rings if necessary

Important output files

IDXREF.LP – the results and data diagnostics of IDXREF

XPARM.XDS – the initial orientation matrix and parameters determined by IDXREF subsequently used in INTEGRATE

INTEGRATE.HKL – the hkl file from INTEGRATE (consequently processed by CORRECT)

INTEGRATE.LP – the results and data diagnostics of INTEGRATE

GXPARM.XDS – the final orientation matrix and parameters determined by CORRECT

CORRECT.LP – the results and data diagnostics of CORRECT

XDS_ASCII.HKL - the final hkl data processed by CORRECT

Remark: it is possible to use the intensities from the file INTEGRATE.HKL for the structure solution/refinement instead of those from the final file XDS_ASCII.HKL. It is especially useful for the high-pressure data.

Things to do before running XDS:

1. Calculate the ROTATION_AXIS using the program phiachse_hasy.pl 2θ ω χ. Put these numbers into XDS.INP. That is: determine the values

   for the input parameters DIRECTION_OF_DETECTOR_X-AXIS, DIRECTION_OF_DETECTOR_Y-AXIS and ROTATION_AXIS.

2. Use the correct DETECTOR_DISTANCE, ORGX and ORGY. You might find these parameters in a powder calibration image, e.g., silicon. ORGX and ORGY could also be determined from the coordinates of the direct beam on the frames.

3. OVERLOAD=50000.

4. FRIEDEL'S_LAW=FALSE

5. FRACTION_OF_POLARIZATION=0.950 (it depends on the radiation and the facility)

6. In case of doubts, check the example of the XDS.INP file in this manual.

XDS procedure for high-pressure data

1. make a new directory (each run requires a separate directory)
2. copy the appropriate input template and rename it XDS.INP
3. put the correct parameters in XDS.INP: ROTATION_AXIS, BACKGROUND_RANGE, SPOT_RANGE, STARTING_ANGLE. Check all the "hardware", distortion, noise, detector position, and incident beam parameters to make sure they are correct.
4. execute XDS (JOB= XDS).
5. check IDXREF.LP that is the result of the indexing.
6. If successful, this step gives you the first complete integration for this data range. If not, see the rest of this manual.
7. cp GXPARM.XDS XPARM.XDS to use optimized input values for the crystal orientation parameters.
8. run XDS for your DATA_RANGE using JOB= INTEGRATE CORRECT.
9. check the 3D profile peak shape in INTEGRATE.LP
10. go to step No. 7.

Things to be careful about to run XDS efficiently with high-pressure data

1. Try to find 2 or 3 frames (BACKGROUND_RANGE) to be used for determining the background with no diamond reflections. You do not have to change them afterwards for integration, etc. The background is determined only once at the beginning and is not updated unlike in other software, e.g., SMART, etc.

2. SPOT_RANGE is used to index the data only and NOT for integrating them. Do not have to change it once the cell is found.

3. STARTING_ANGLE corresponds to the first frame in SPOT_RANGE and NOT to the first frame in your run. **NEVER** change it after indexing!!!! We always choose the same 20-30 frames for the SPOT_RANGE and the initial DATA_RANGE from the middle of the run, i.e., when the diamond anvil cell is (nearly) perpendicular to the direct beam and the shadowed areas of the detectors are small.

4. Once the data are ready for integration, only change the DATA_RANGE expanding it by a few frames on both ends. The most effective total number of frames added is lower than the DELPHI parameter providing that OSCILLATION_RANGE= 1.0. This will make sure that the orientation matrix is not messed up when the integration goes awry.

5. Good integration requires several XDS runs and checking the peak shape in INTEGRATE.LP each time.

6. Always run CORRECT with space group no. 1 for the high-pressure data even though you are absolutely sure of the exact symmetry. Check your XDS.INP as well as GXPARM.XDS and XPARMS.XDS files and put it back to 1 when higher symmetry is found! Otherwise, CORRECT will perform corrections and data averaging that depend on the space group symmetry and will yield disastrous intensities. In any case, it is possible to use the intensities from the INTEGRATE.HKL file for the structure solution/refinement instead of those from the final file XDS_ASCII.HKL. The only really useful information from CORRECT is about the ESDs of the lattice parameters.

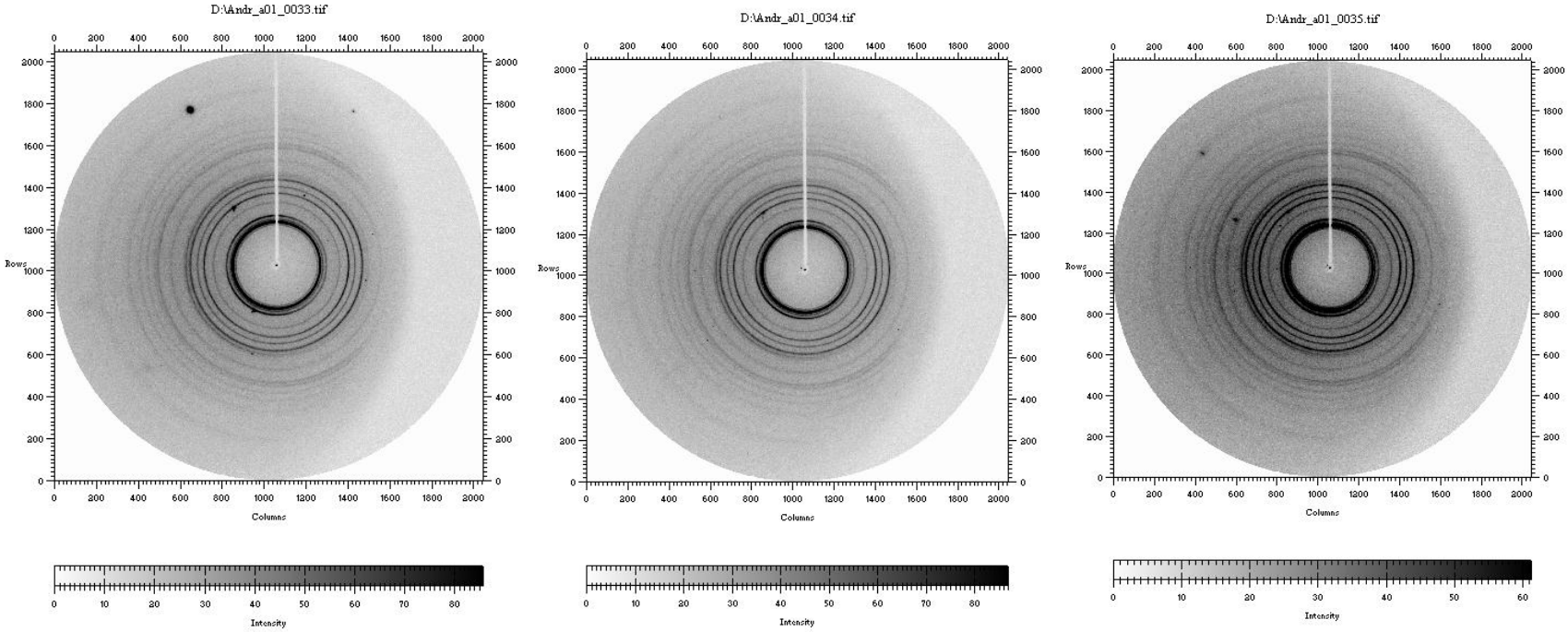
Warning: XDS remembers what it did by using input information from the file XPARM.XDS too. Hence, when you have to restart it from scratch, for instance in case the indexing has failed (see below), always delete all the files (except for XDS.INP) from your working directory first.

Some issues to know about:

- Background
- Indexing
- Integration
- Corrections

Background

Our experience with the high-pressure data from marCCD165 tells us that the best way to determine the background is to use data images without strong diamond reflections. The following three frames are considered to be OK.



When using XDS, the most difficult task is to index the high-pressure data. Once the cell is found, the rest is easy!

The most common reasons for failing to index high-pressure data in the default run of XDS are wrong input parameters, crystal misalignment, and/or the presence of *alien* spots arising from diamond reflections and gasket rings. Providing the input parameters are correct and the crystal is well aligned, the error message at the end of the run in the file IDXREF.LP nearly always is: INSUFFICIENT PERCENTAGE (<50%) OF INDEXED REFLECTIONS. The program just complains that less than 50% of spots could be indexed, although the cell is correct. To proceed, the line "JOB = DEFPIX INTEGRATE CORRECT" has to be used and XDS rerun. If you get any other error message, it means that (1) something must be wrong with the input parameters, diffractometer, and/or crystal, (2) there are just too many spurious reflections (spots due to the gasket, for instance) and XDS fails. In the latter case, the trick is to delete the weakest spots from the SPOT.XDS file (for instance those with their intensities below 3) and run XDS with the command "JOB = IDXREF DEFPIX XPLAN INTEGRATE CORRECT". The most likely result ends with the message "INSUFFICIENT PERCENTAGE (<50%) OF INDEXED REFLECTIONS". If this does not work, you could try changing the SPOT_RANGE. By the way, the spots from diamonds, which are the strongest, normally do not cause any problems as there are too few of them. Of course, they could also be deleted (their intensities are usually very high) before running XDS with JOB = IDXREF DEFPIX XPLAN INTEGRATE CORRECT.

The orientation matrix is in the direct space. It refers to the spindle position at the start of the first spot range frame (STARTING_ANGLE) and *not to the true spindle dial setting* (see the files XPARM.XDS and GXPARM.XDS).

If it happens that your material has undergone a phase transition and you have no idea about the lattice, you could use the following entries in the file XDS.INP (please note the ! exclamation signs):

```
!SPACE_GROUP_NUMBER=     1
!UNIT_CELL_CONSTANTS=    7.5 8.5 5.7 90.0 90.0 90.0
```

This procedure is equivalent to the parameter:

```
SPACE_GROUP_NUMBER=     0
```

In this case, the line with UNIT_CELL_CONSTANTS is ignored.

If you know the lattice, you use these parameters without the "!" exclamation signs and a set of approximate lattice parameters. Remember that the space group has to be always No. 1 for high-pressure studies:

```
SPACE_GROUP_NUMBER=     1
```

Another trick is to use the (approximate) components of the unit-cell basis vectors with respect to the laboratory coordinate system for the unrotated crystal specified by the parameters UNIT_CELL_A-AXIS, UNIT_CELL_B-AXIS, and UNIT_CELL_C-AXIS.

Integration

The spots are described as Gaussians with four parameters BEAM_DIVERGENCE, BEAM_DIVERGENCE_E.S.D., REFLECTING_RANGE, and REFLECTING_RANGE_E.S.D. If any of them is unspecified, its value is determined automatically from the data images (the learned reflection profiles). These parameters are optimized during each integration.

The INTEGRATE subroutine generates profile templates for the reflections within the DATA_RANGE and DELPHI parameters (the profile templates are explained in the XDS manual http://xds.mpimf-heidelberg.mpg.de and in the XDS publications in Acta Cryst. D). They are shown in the diagnostics file INTEGRATE.LP and should look more or less like this (sequence of blocks 1 to 9 follow the rotation of the crystal, central point in block 5 = 100, block 5 with a border of zeros, block 1 = block 9: only zeros):

```
 0  0  0  0  0  1  0  0  0     0  0  0  0  1  1  0  0  0     0  0 -1 -1  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  1  0  0
 0  0  0  0  0  0  0  0  0     1  0  0  1  0  0  0  0  0     0  0  0  1  2  1  1  0  0
 0  0  0  0  0  0  0  0  0     0  0  0  1  2  0  0  0  0     0  0  1  5 12  5  1  0  0
 0  0  0  0  0  0  0  0  0     0  0  0  2  4  2  0  0  0     0  0  1 10 26 10  1  0  0       block 1 2 3
 0  0  0  0  0  0  0  0  0     0  0  0  1  2  1  0  0  1     0  0  1  5 12  5  1  0  0
 0  0  0  0  0  0  0  0  0     0  0  0  0  0  0  0  0  0     0  0  0  1  2  1  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  1  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 -1  0  0  1  1  0  0     0  0 -1  0  1  1  2  0  0     0  0 -1  0  1  0  1  0  0
 0  0 -1  0  1  1  1  0  0     0  0 -1  0  2  1  1  1  0     0  0 -1  0  1  0  1  0  0
 1  0  1  4  6  3  1  0 -1     1  0  1  5  8  4  1  0 -1     1  0  1  3  6  3  1  0 -1
 0  0  3 15 32 14  2  0 -1     1  1  3 20 46 20  3  0 -1     1  1  2 14 32 14  2  0 -1
 0  0  4 26 70 28  3  0  0     0  0  5 37100 40  4  0  0     0  0  4 26 70 28  2  0  0       block 4 5 6
-1  0  2 13 32 14  2  0  0    -1  0  3 18 45 20  2  0  0     0  0  2 13 32 14  2  0  0
-1 -1  1  3  4  2  0  0  0    -1 -1  2  4  6  3  0  0  0    -1  0  1  3  4  2  0  0  0
 0 -1 -1  1  1  0  1 -1  0     0 -1 -1  1  1  0  1 -1  0     0  0  0  1  1  0  1 -1  0
 0  0  0  0  0 -1  0  0  0     0  0  0  0 -1 -1  0  0  0     0  0  0  0 -1 -1  0  0  0

 0  0  0  0  0  0  0  0  0     0  0 -1  0  0  0  0  0  0     0  0 -1  0  0  0  0  0  0
 0  0  0  0  0  0  0  2  0     0 -1  0  0  0  0  0  1  0     0 -1  0  0  0  0  0  0  0
 0  0  0  1  2  1  0  0 -1     0  0  0  0  0  0  0  0  0     1  0 -1  0  0  0  0  0  0
 0  1  1  5 12  5  0  0 -1     0  0  0  1  2  1  0  0  0     1  0  0  0  1  0  0  0  1
 0  0  1  9 25 10  1  0  0     0  1  1  2  4  2  0  0  0     1  0  0  0  1  0  0  0  0       block 7 8 9
 0  0  1  4 12  5  0  0  0     0  0  1  1  2  1  0  0  0     1  0  1  1  0  1  0  0  0
 0  0  1  1  2  1  0  0  1     0  0  0  0  0  0  0  0  0     0  0  0  0  0  0  0 -1  0
```

```
 0  0  0  0  0  0  1  0  0     0  0  0  0  0  0  0  0  0     0  0  0  0  0 -1  0 -1  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
```

Off-centered profiles (e.g., the number 100 is not exactly in the middle) indicate an unrefined or wrong orientation matrix, misindexing, crystal decentering, etc. The profiles extending to the borders of the box indicate wrong BEAM_DIVERGENCE, BEAM_DIVERGENCE_E.S.D., REFLECTING_RANGE, and REFLECTING_RANGE_E.S.D. parameters. A suggestion for their optimized values is given in the file INTEGRATE.LP (in this file they are called "SUGGESTED VALUES FOR INPUT PARAMETERS"). Start with small values for these parameters and increase them as indicated by the profiles in INTEGRATE.LP. In any case, the "suggested" profile parameters are not always correct, especially when the reflections from your crystal overlap with those from diamonds and with the Debye-Scherrer gasket rings.

To get the profiles right, you need to run INTEGRATE several times. Also important is the refinement of the lattice parameters within the data image range specified by the DELPHI parameter. If it does not converge, you have a problem similar to profiles being off-centered.

Corrections

The errors in the lattice parameters are given in the file CORRECT.LP. That is the only information we are going to use from the CORRECT step.