ABSORB

Ross Angel
and
Javier Gonzalez-Platas

And with a lot help from Andrzej among many others including Charlie Burnham and Larry Finger!

- ***Implementing absorption corrections with a physical basis***
  - ***X-rays only***
  - ***DACs***
- ***Go through the issues and illustrate how to do it in ABSORB***

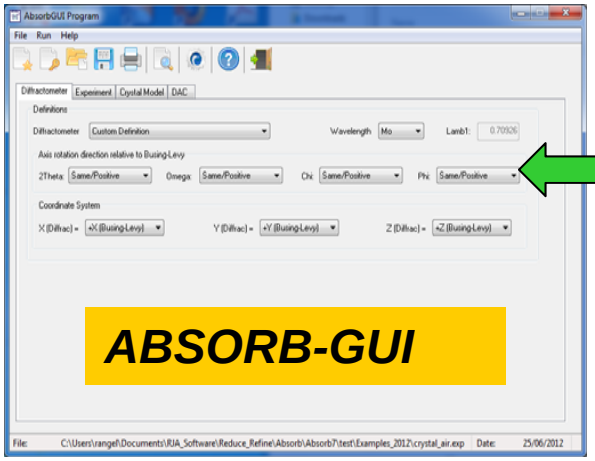
ABSORB 7

- **ABSORB has been developed for 50 years!**
  - **Which makes it older than the operating systems!**
  - **Originally a program for crystals in air (Burnham, 1966)**
  - **Some development for DACs (Finger 1970s, 80s)**
  - **Further development for DACs and special cases (Angel, 2004)**
  - **Absorb controlled by text files**

- **ABSORB-7 and ABSORB-GUI**
  - **Angel and Gonzalez-Platas (2012)**
  - **Separation of Absorb 'engine' and input**
  - **Allows direct integration in to commercial software**
  - **GUI for stand-alone users.**

- **ABSORB-7 remains a research tool**
  - **Lots of options**
  - **And some weird stuff (thanks to Clivia!)**

ABSORB workflow



ABSORB-GUI

Experiment file

Text editor

Commercial software

Intensity data file

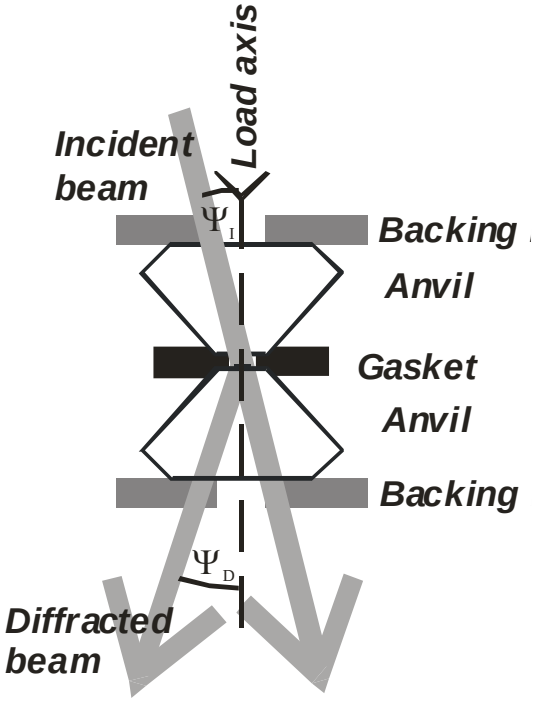
ABSORB-7 engine

Corrections file
Print file
cif

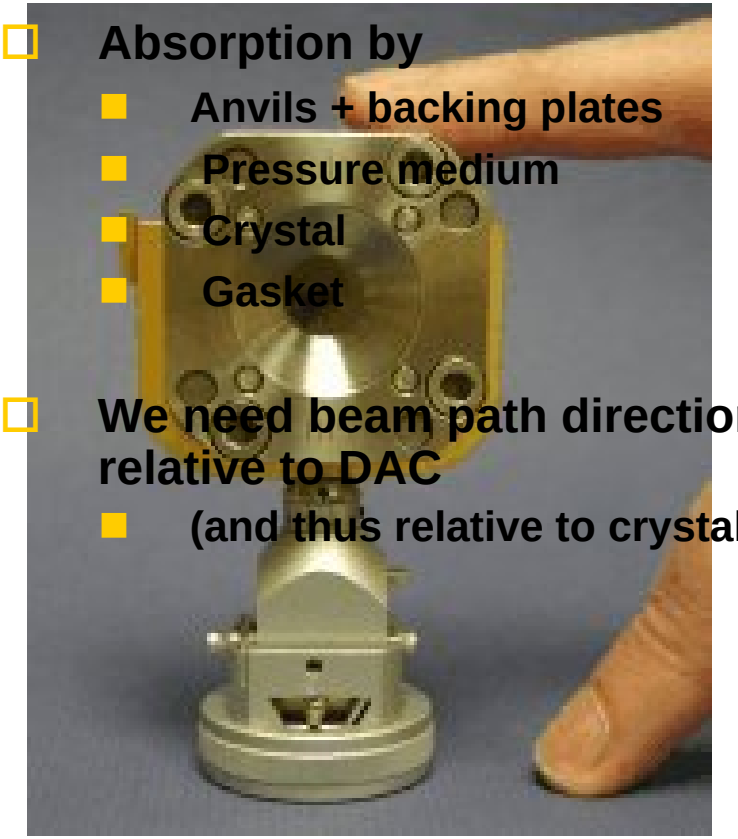
Corrected data file

Averaging and refinement

Absorption in the DAC: geometry

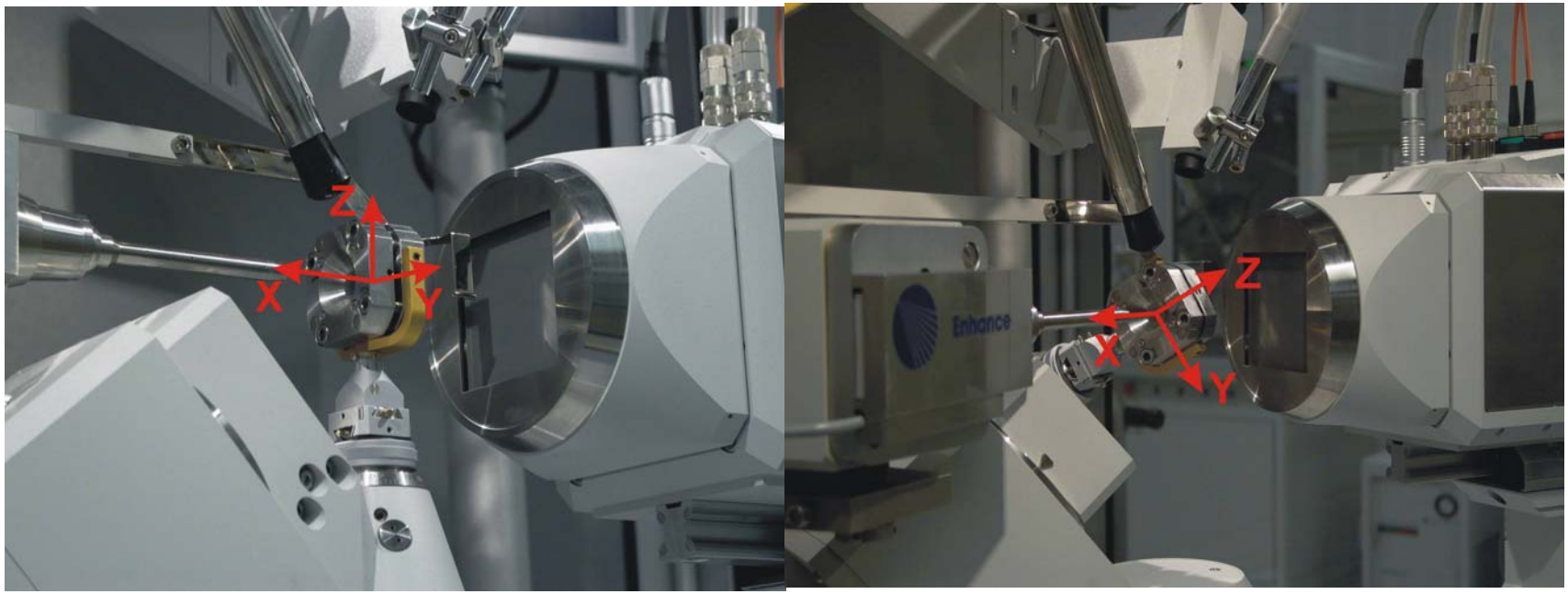


Transmission mode



- Absorption by
  - Anvils + backing plates
  - Pressure medium
  - Crystal
  - Gasket
- We need beam path directions relative to DAC
  - (and thus relative to crystal as well)

Absorption in the DAC: defining beam paths



- The DAC is fixed to the goniometer head
- A natural Cartesian reference basis is therefore a basis fixed to the goniometer head (phi-axis system)
- Define beam paths on this axial system

Busing, Levy (1967) Acta Cryst 22:457

Defining beam paths in SHELX hkl files

Direction cosines of I-beam and D-beam

- relative to crystal reciprocal axes
- Works for any detector type
- Only snag is absolute orientation of crystal not specified
- Requires UB matrix for conversion to phi-axis

example234.hkl - Notepad

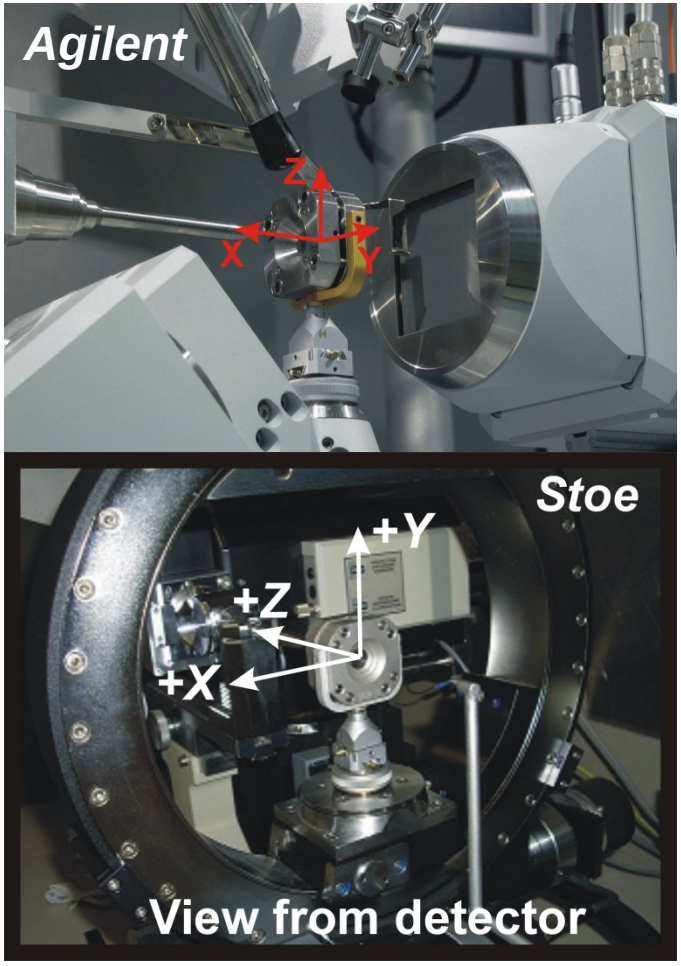
File Edit Format View Help

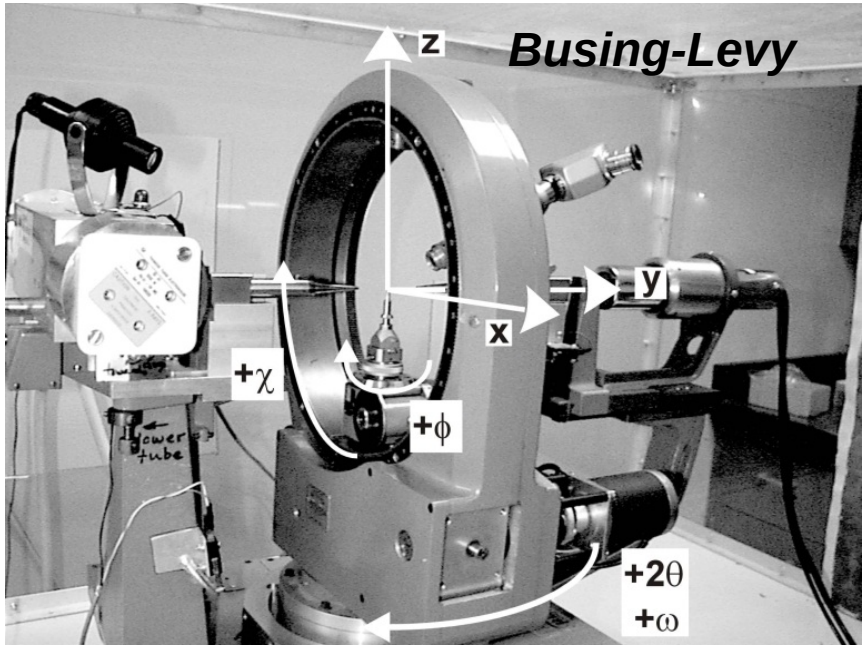
```
  -6    1    0 5.79738 0.31172    1-0.23997-0.53208 0.97037-0.84621 0.02801-0.02828
  -6    0    0 1069.78 22.2590    1-0.38709-0.38476 0.92172-0.92267 0.02437-0.02457
  -6    0    1 0.00000 0.97044    1-0.38537-0.38646 0.92012-0.92208 0.06957 0.02019
  -6    0    2 486.681 9.87660    1-0.38113-0.39070 0.91738-0.91820 0.11445 0.06531
  -6    0    3 0.00000 1.04327    1-0.37941-0.39243 0.91128-0.91321 0.15981 0.10988
  -6    0    4 910.872 18.8337    1-0.37516-0.39668 0.90412-0.90472 0.20423 0.15545
  -6   -1    4 0.30345 0.05248    1-0.52157-0.25023 0.82945-0.95490 0.19968 0.16005
  -6   -1    3 1.84826 0.12085    1-0.52550-0.24621 0.83652-0.96241 0.15495 0.11481
  -6   -1    2 20.2423 0.58635    1-0.52868-0.24304 0.84164-0.96751 0.10998 0.06983
  -6   -1    1 7.39602 0.38137    1-0.53164-0.24006 0.84446-0.97044 0.06500 0.02484
  -6   -1    0 6.07595 0.31568    1-0.5342[illegible]                0.01995-0.02011
  -6   -2    0 746.423 14.6594    1-0.6690[illegible]                0.01519-0.01530
  -6   -2    1 21.5116 0.56781    1-0.6668[illegible] 0.74271-0.9940[illegible] 0.06024 0.02964
  -6   -2    2 391.931 7.67619    1-0.66421-0.10732 0.74007-0.99144 0.10526 0.07458
```

$h\phi = UB.h$

Phi-axis definitions

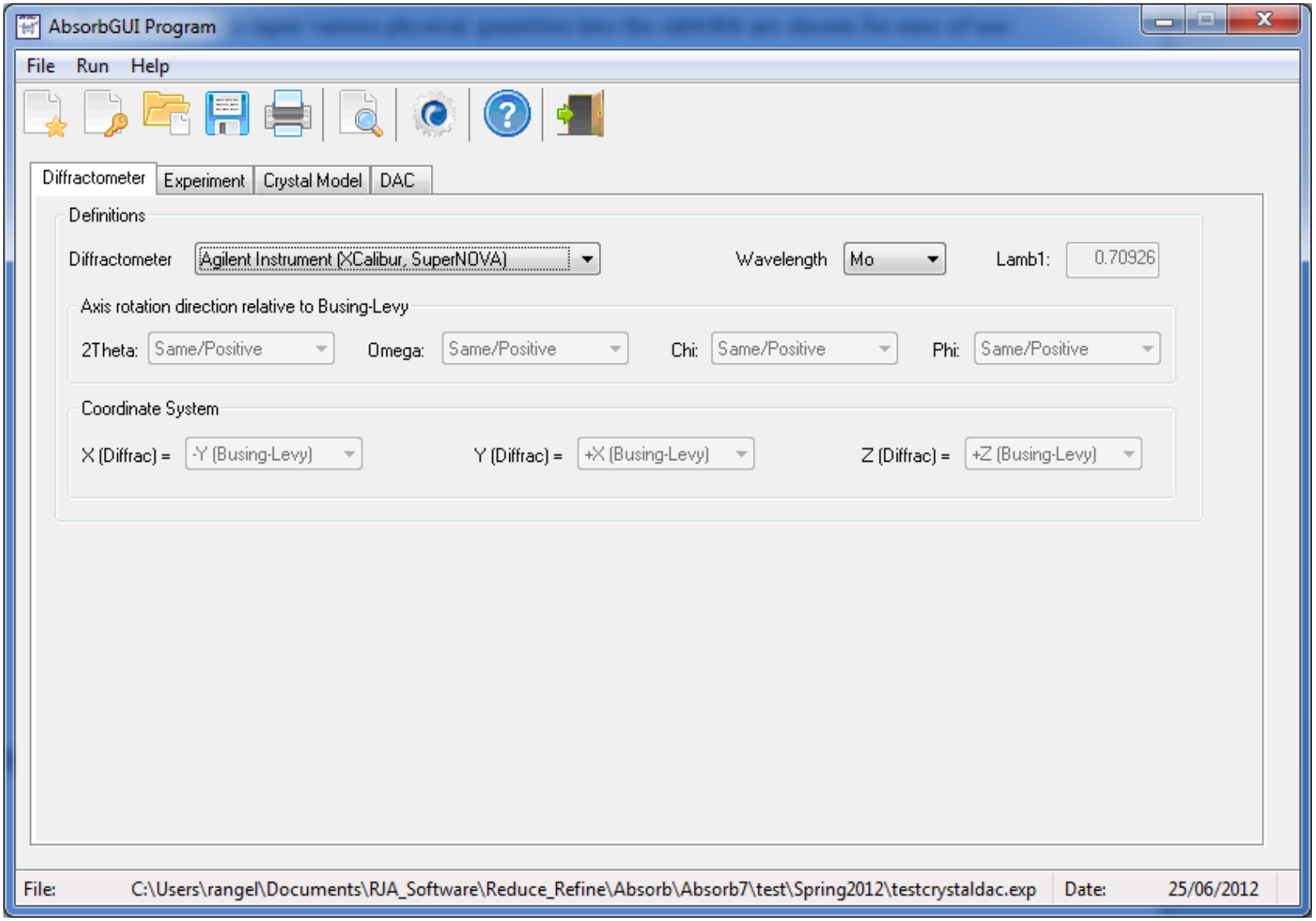
- **The definition of the phi-axis system, and thus U and UB, is different in different software!**
  - **Axis directions when diffractometer circles at zero**



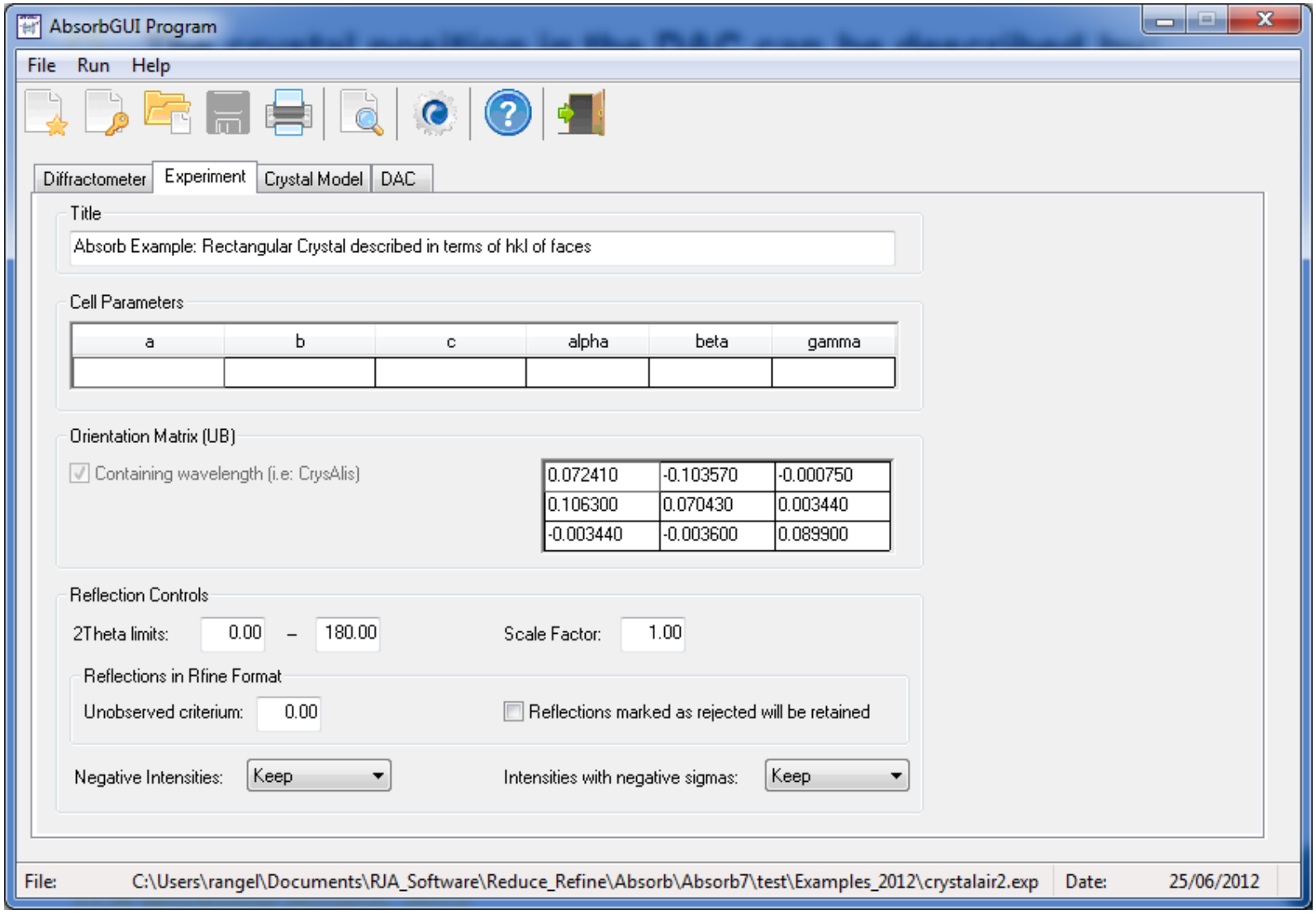


- ***ABSORB works in Busing-Levy***

Diffractometer parameters



And the UB matrix can now be given



DAC Absorption

Backing

Anvil

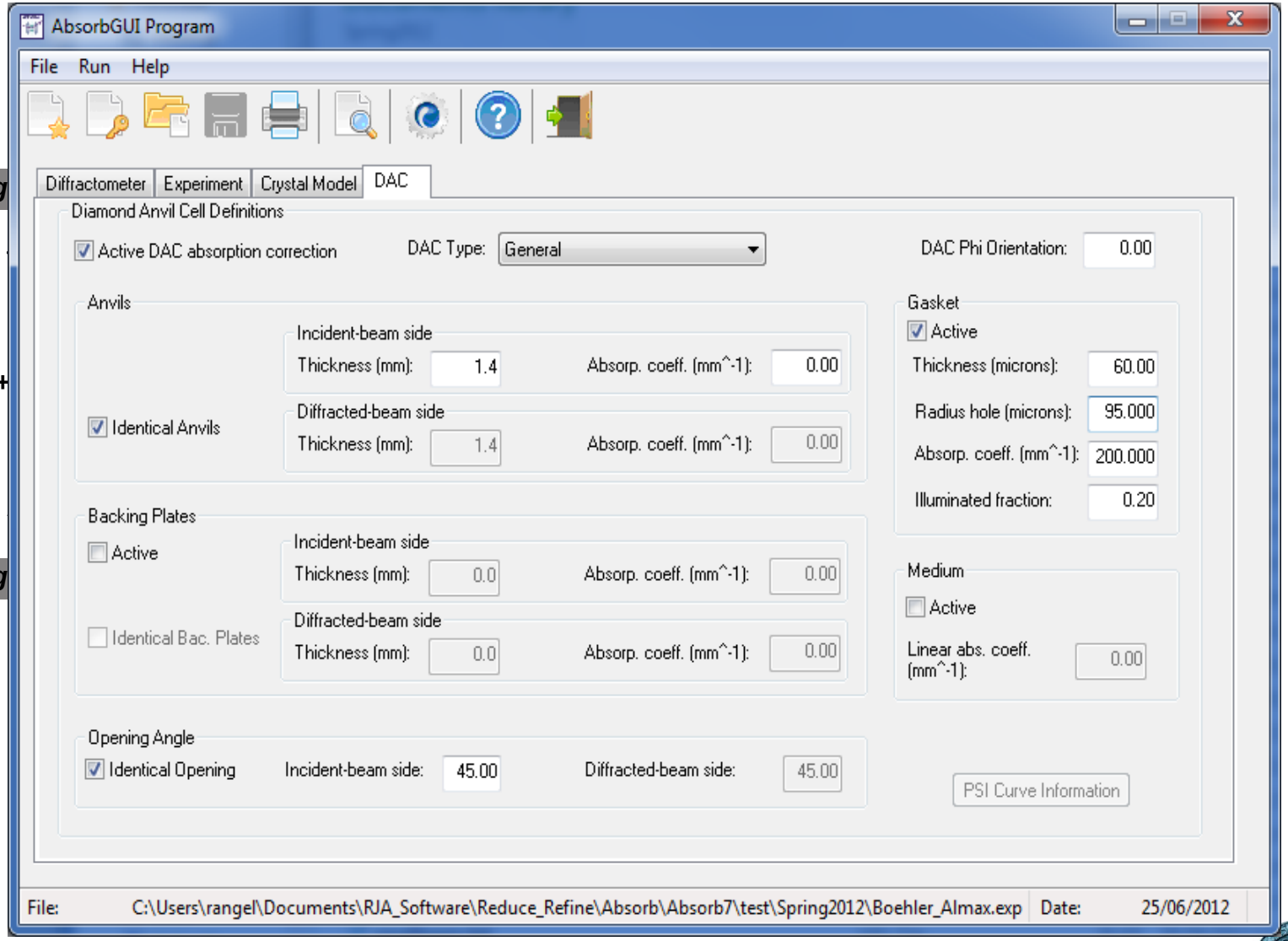
Gasket

Crystal+

Gasket

Anvil

Backing



DAC with beryllium seats

AbsorbGUI Program

File Run Help

Diffractometer | Experiment | Crystal Model | DAC

correction

DAC Type: General

DAC Phi Orientation: 0.00

Incident-beam side
Thickness (mm): 1.4 Absorp. coeff. (mm^-1): 0.00

Diffracted-beam side
Thickness (mm): 1.4 Absorp. coeff. (mm^-1): 0.00

Incident-beam side
Thickness (mm): 4.0 Absorp. coeff. (mm^-1): 0.00

Diffracted-beam side
Thickness (mm): 0.0 Absorp. coeff. (mm^-1): 0.00

Incident-beam side: 40.00 Diffracted-beam side: 45.00

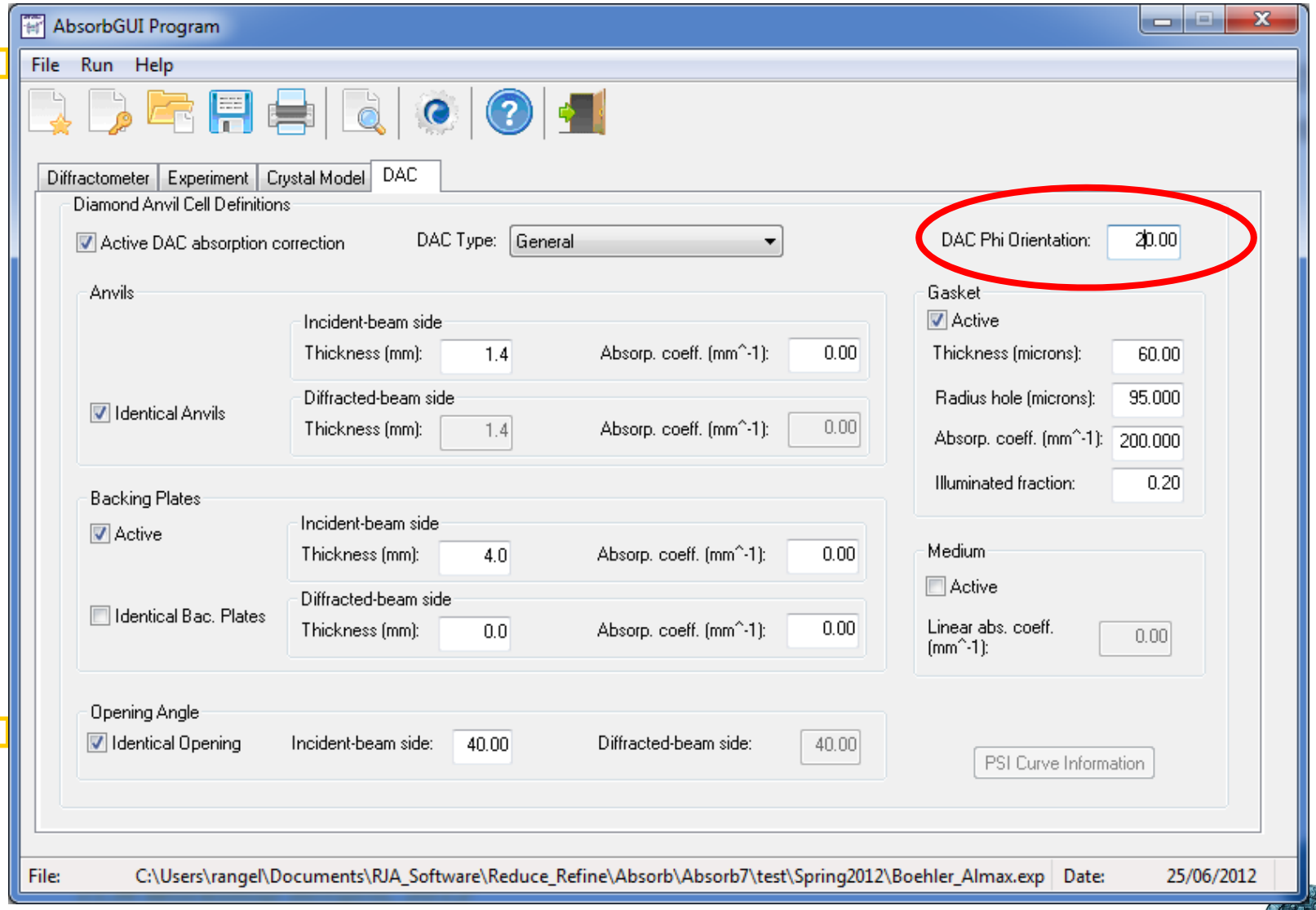
Gasket
Active
Thickness (microns): 60.00
Radius hole (microns): 95.000
Absorp. coeff. (mm^-1): 200.000
Illuminated fraction: 0.20

Medium
Active
Linear abs. coeff. (mm^-1): 0.00

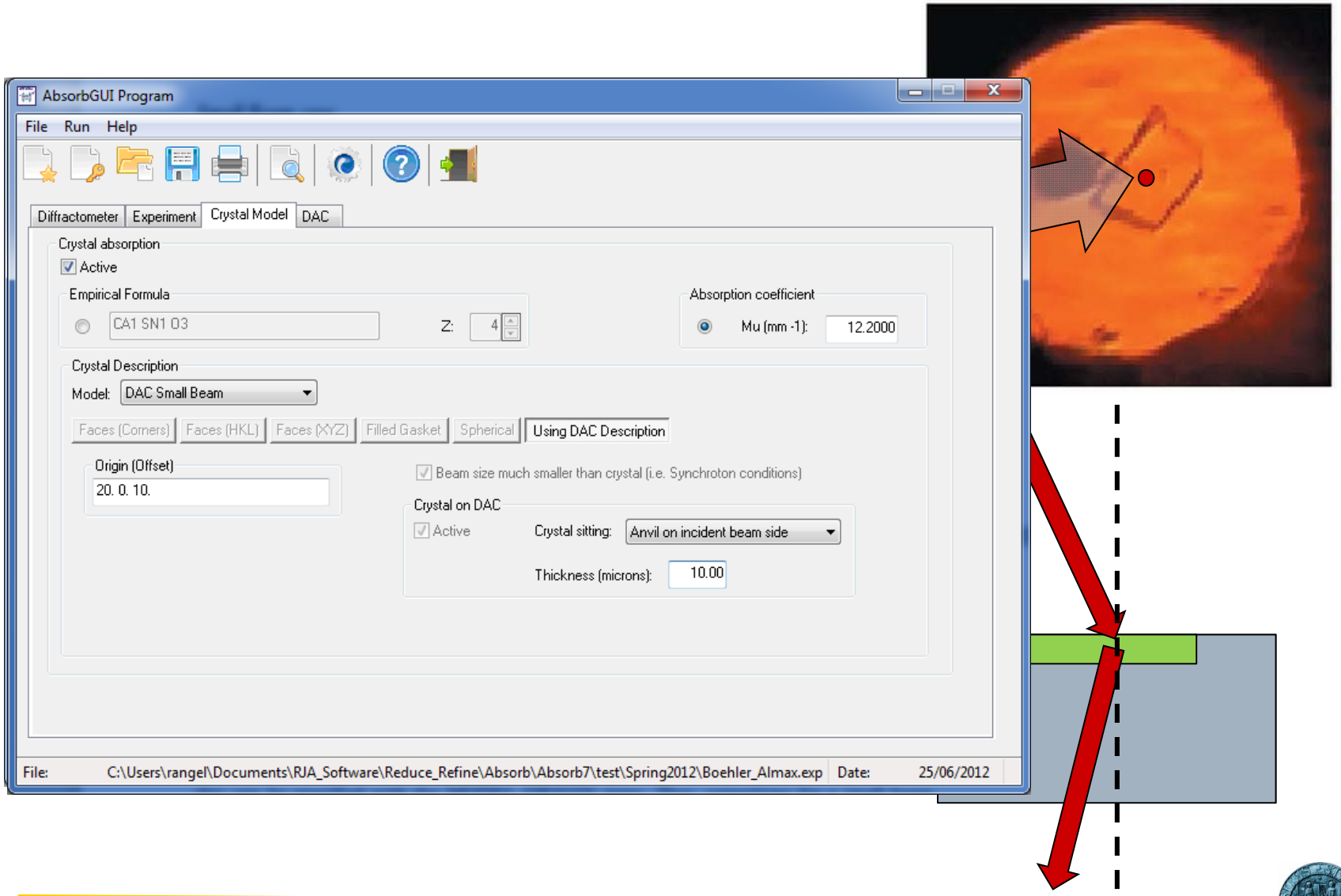
PSI Curve Information

File: C:\Users\rangel\Documents\RJA_Software\Reduce_Refine\Absorb\Absorb7\test\Spring2012\Boehler_Almax.exp Date: 25/06/2012

The DAC on the goniometer



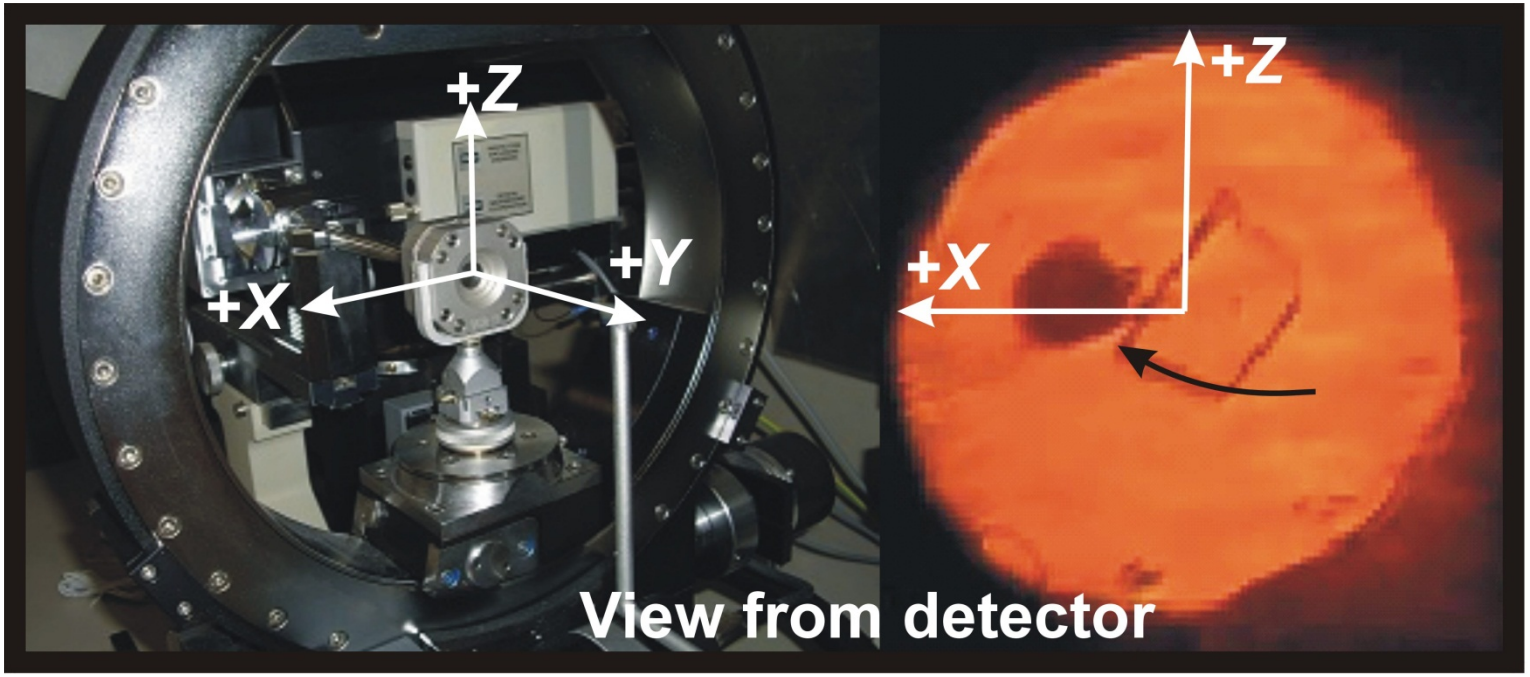
Small beam case



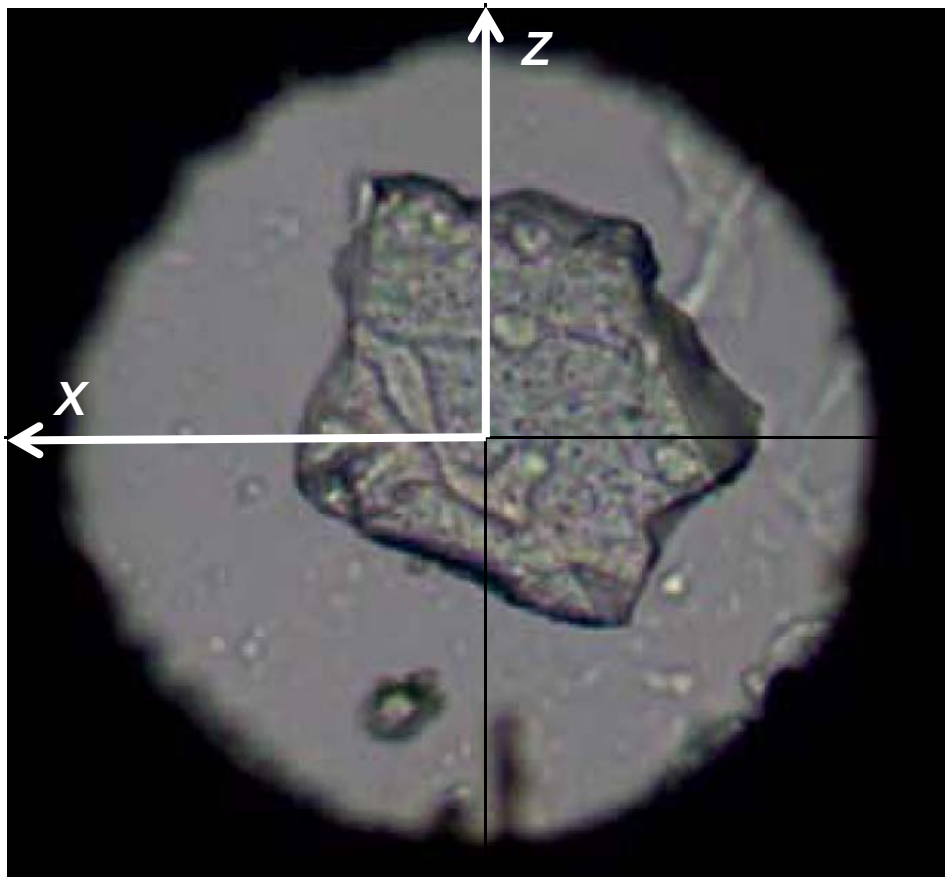
Describing the crystal

- The crystal position in the DAC can be described by:
  - The Miller indices and distances of faces
  - Coordinates of the corners

- In addition, the position of the crystal relative to the gasket centre must be defined for gasket shadowing:

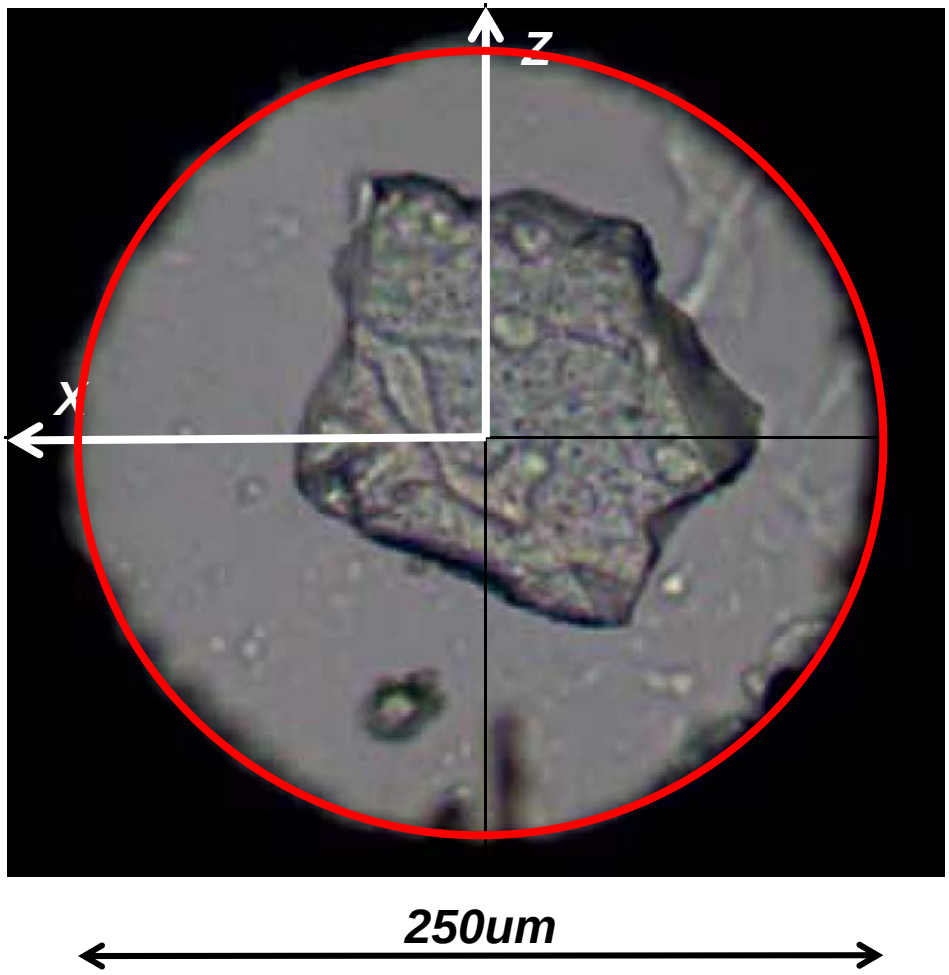


Measuring the crystal



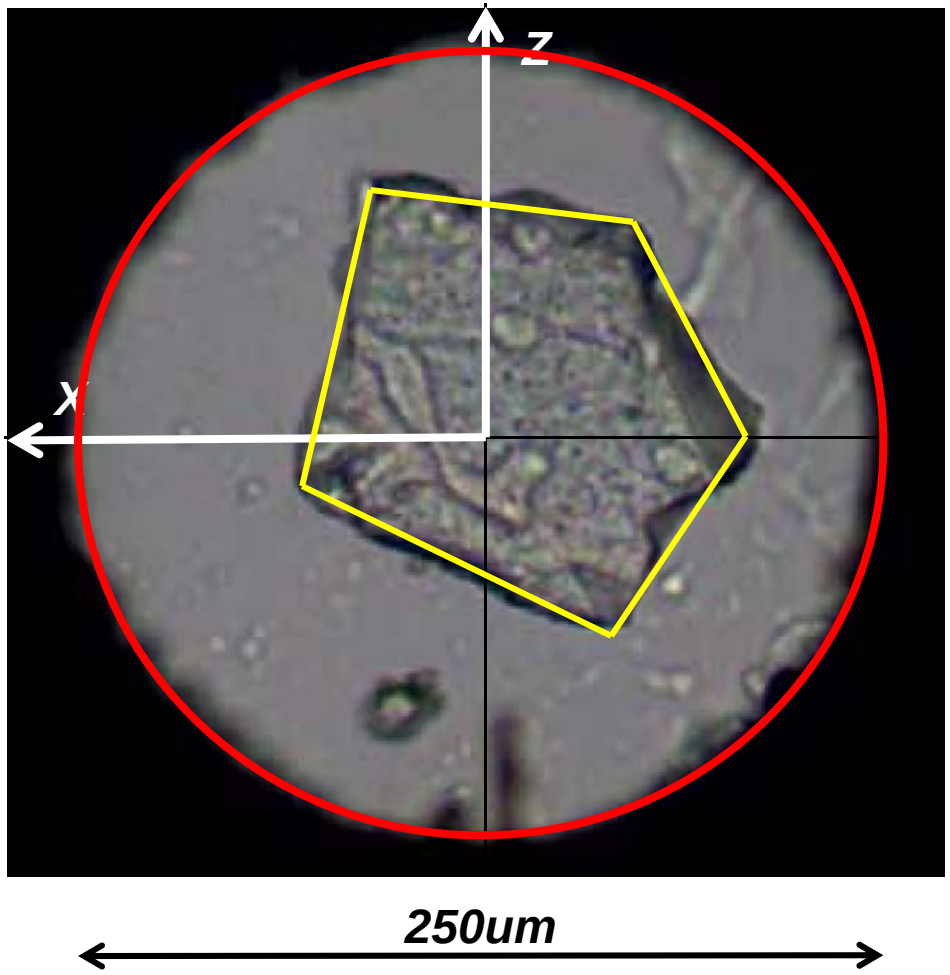
- Capture an image
- Beware of optical inversion and rotation!
- View from which side?
  - Write it down!!!
  - Name the file!!!
- This is the real view from detector side

Measuring the crystal



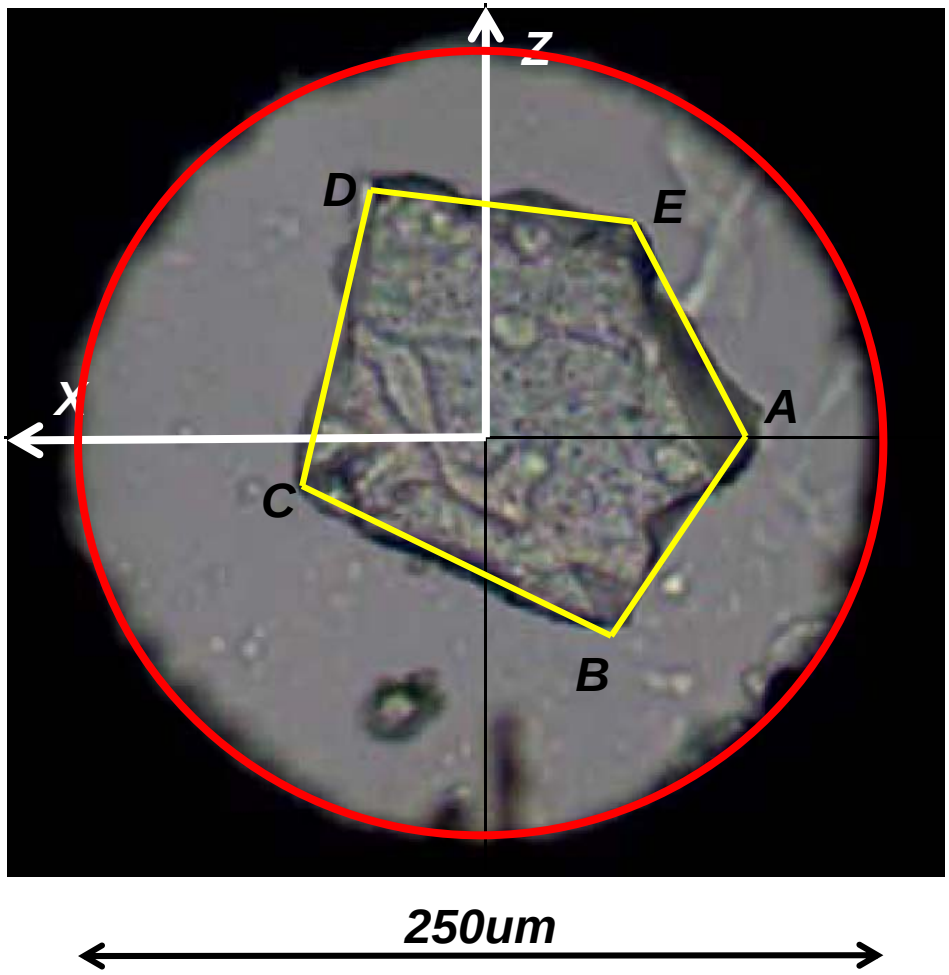
- The gasket gives you a length scale

Measuring the crystal



- Make a simple representation of the crystal
  - Using Gaussian grid
  - Must be convex

Measuring the crystal

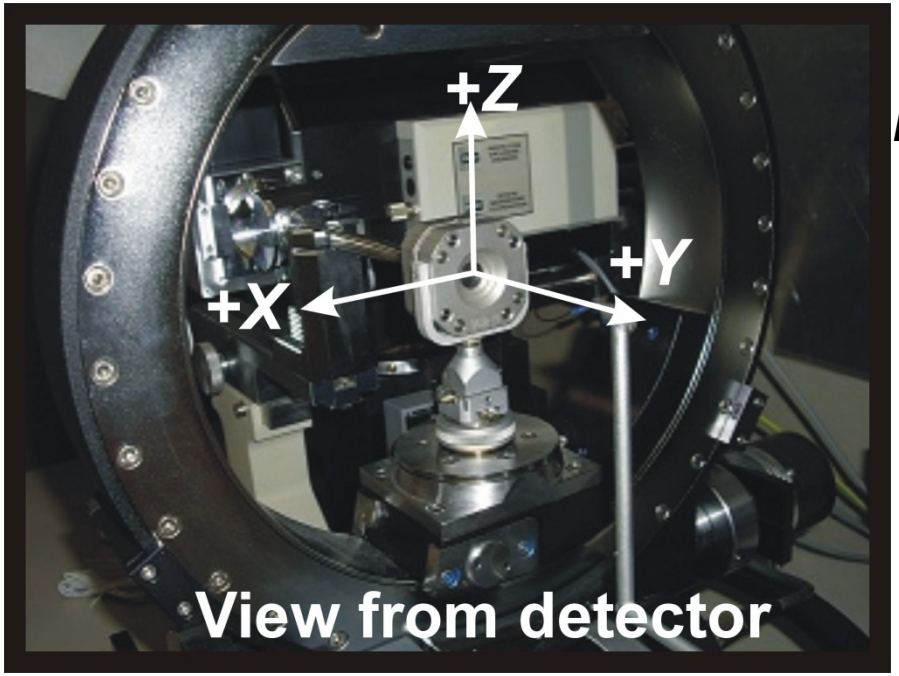


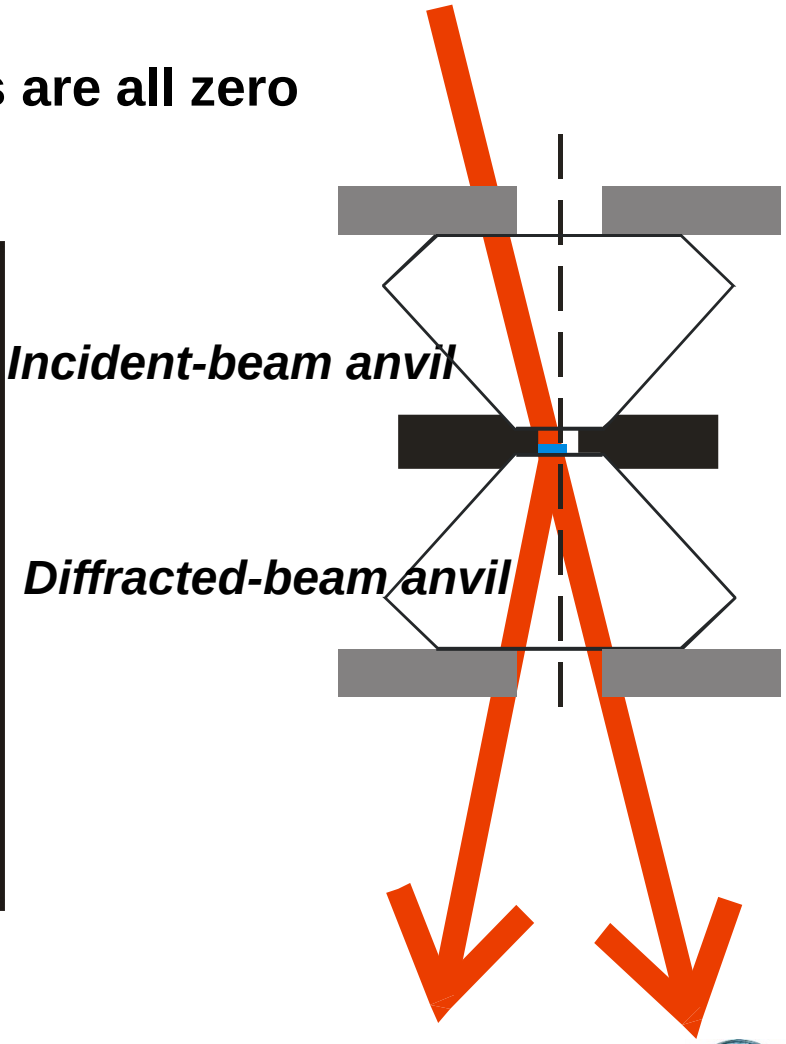
- Measure the x,z coordinates of corners
- Scale from gasket to convert to um:

	x	z
A	-82	0
B	-38	-63
C	+58	-14
D	+36	+77
E	-48	+67

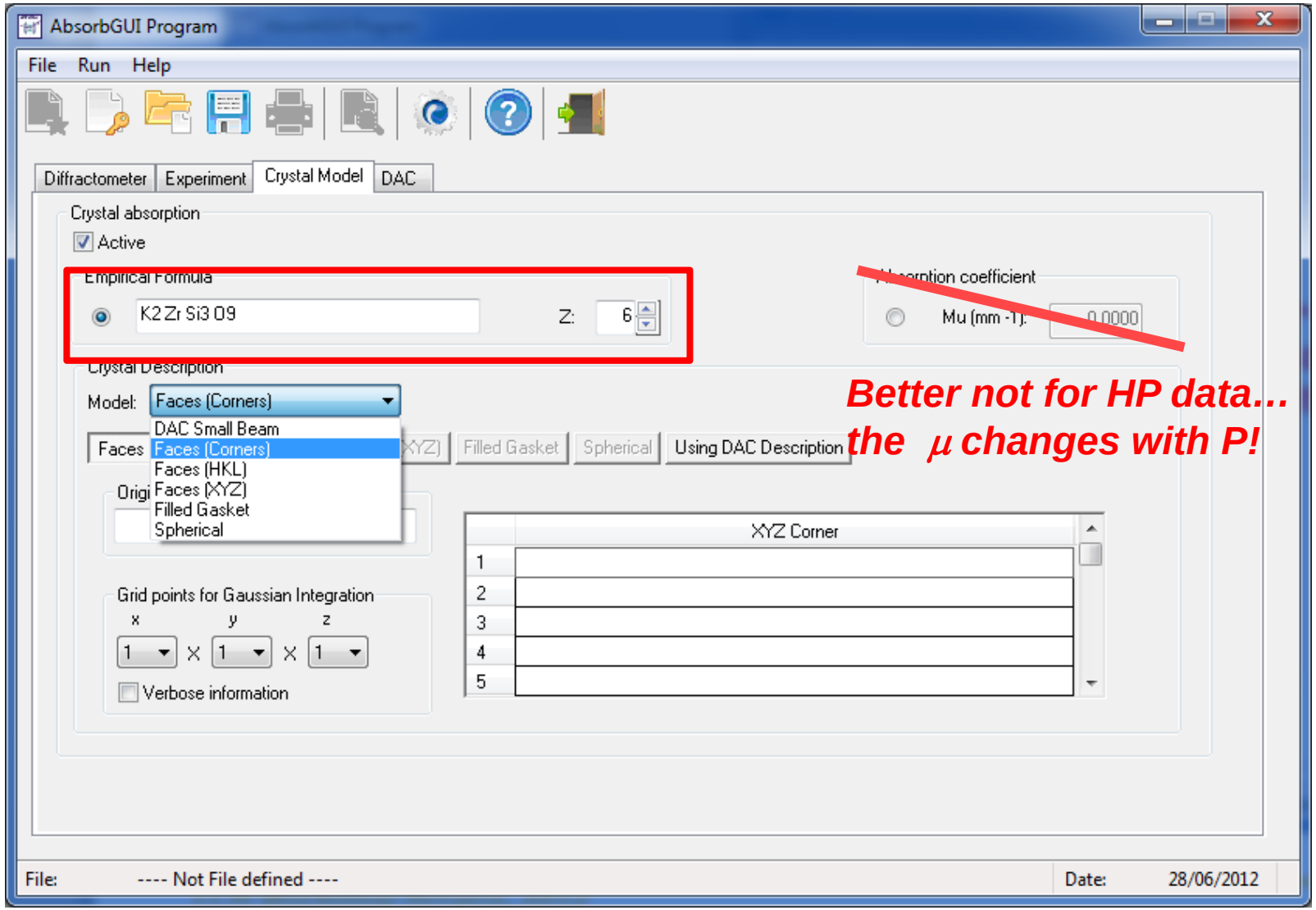
Measuring the crystal

- Y-coordinates: Which anvil?
- When the diffractometer angles are all zero



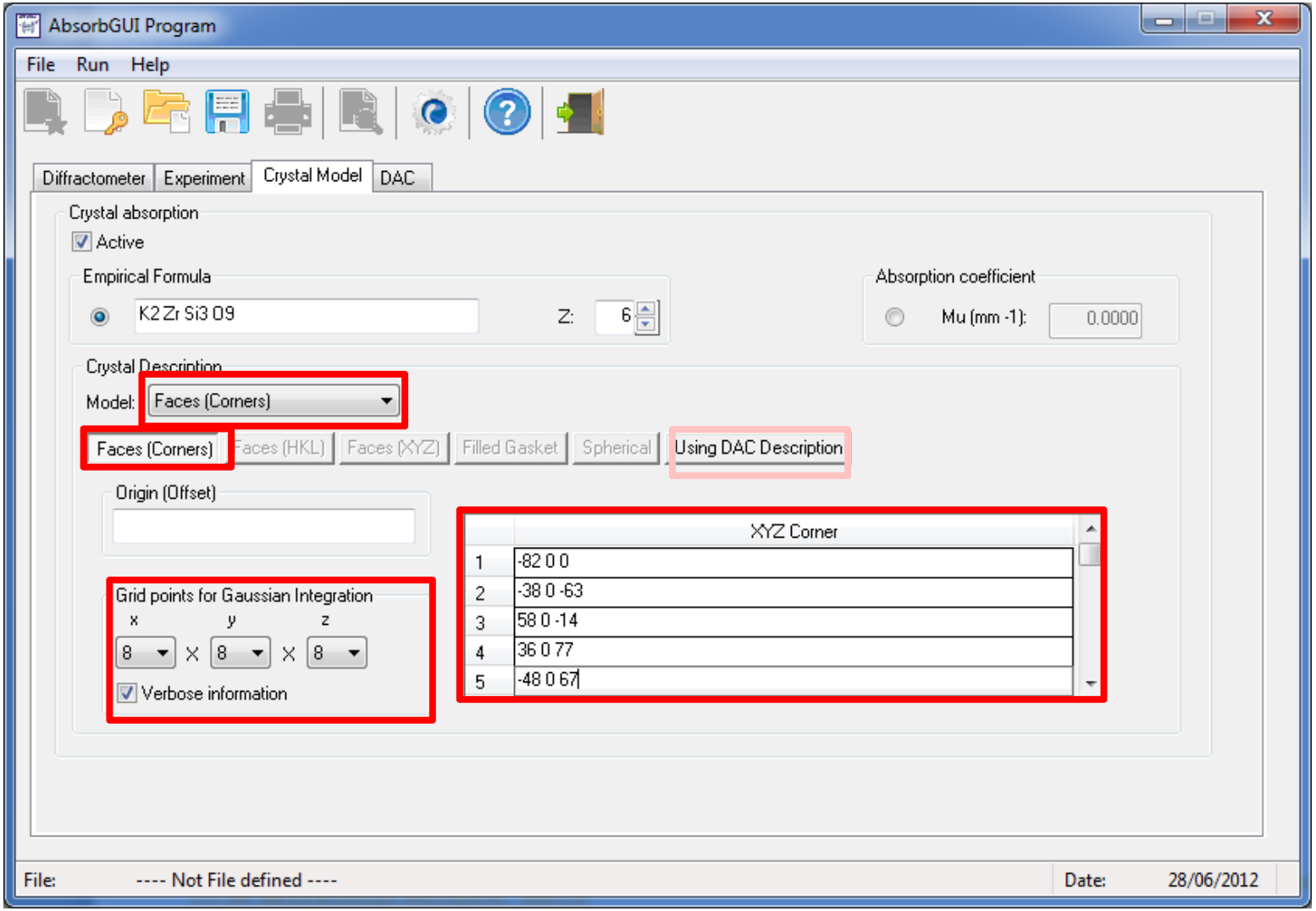


Now load the crystal information

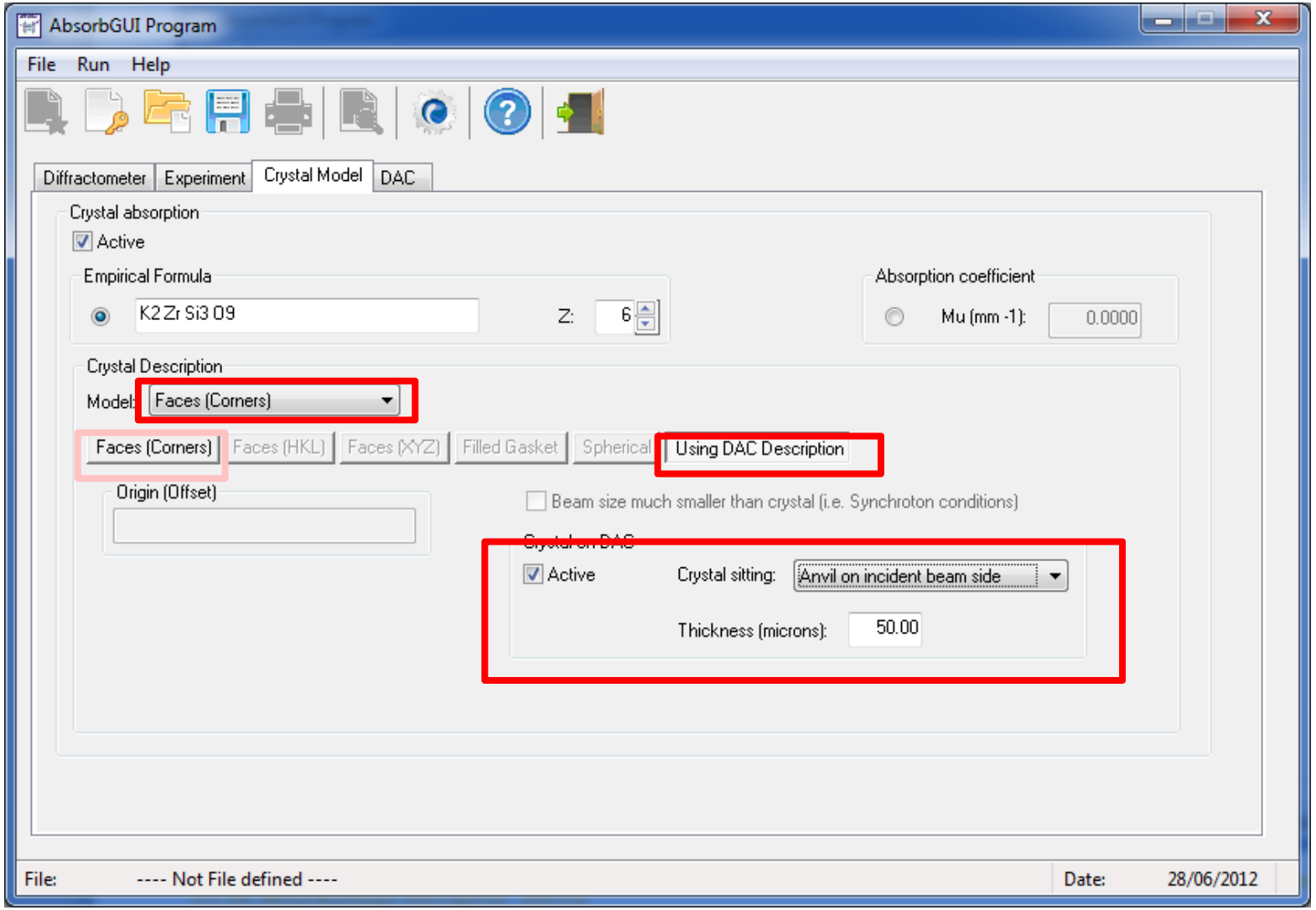


Better not for HP data… the μ changes with P!

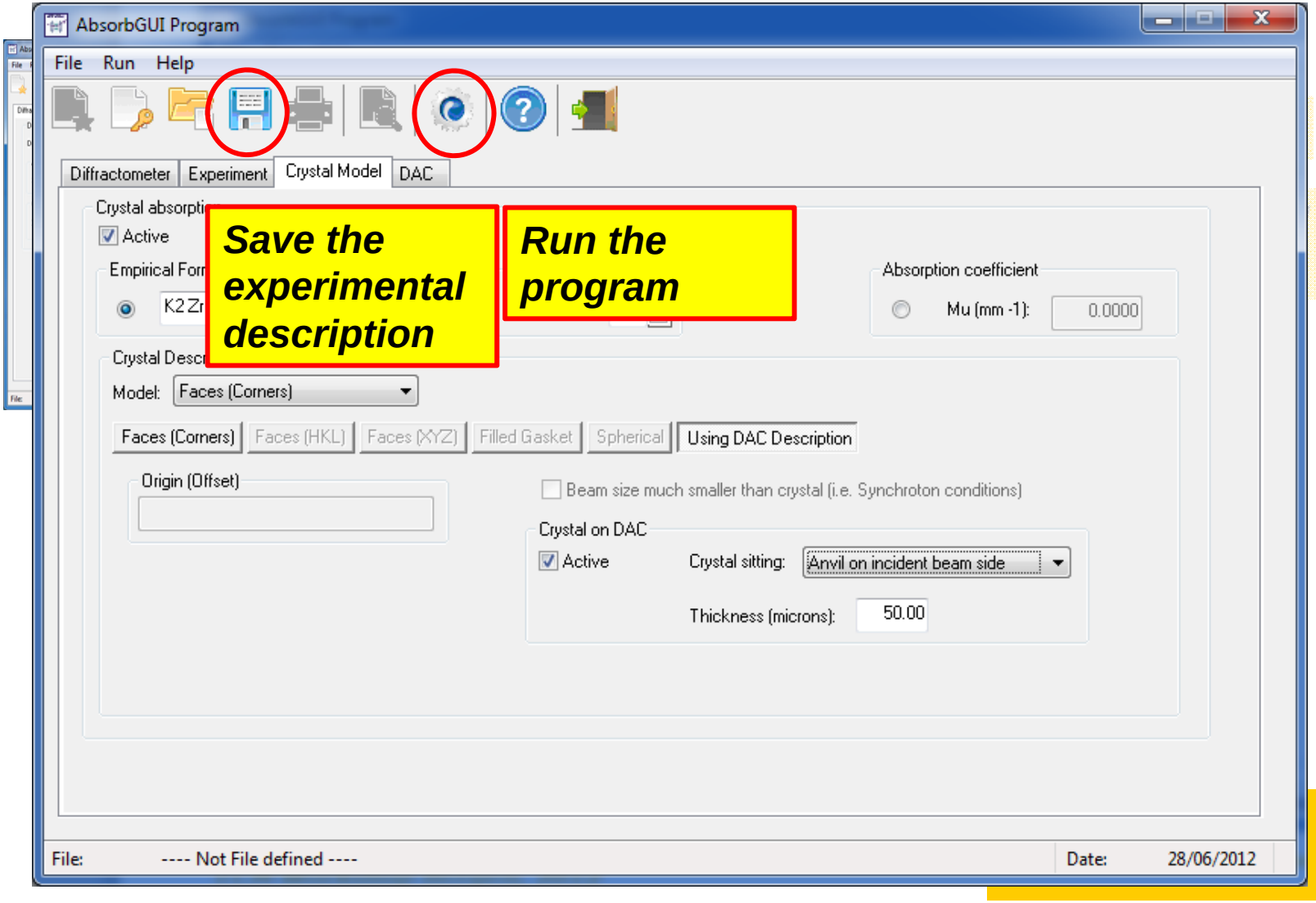
Now load the crystal information



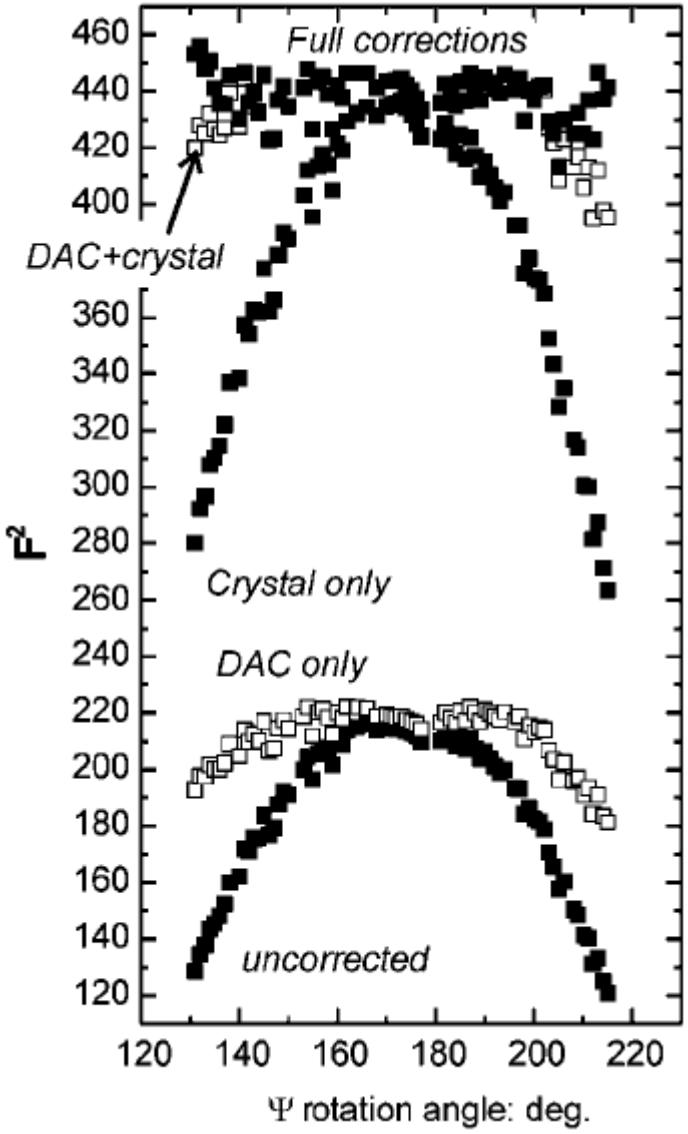
Now load the crystal information



Ready to run the program



Test models with psi scans or equivalents



Other DAC options

- PD data
  - Setting angles in file
  - Parities
  - No UB
- Crystal
  - Co-ords of corners
- DAC description
  - Transmission curve
  - Gasket

DAC_psiscan.exp - Notepad

File Edit Format View Help

```
#
# Experimental File using AbsorbGUI Program
#
TITLE Absorb Example: Psiscan data of a crystal in DAC

# Diffractometer Information
WAVEL    1   0.70926
PARITY      1   1   1   1
BLAXES      1   2   3

# Experimental Information
CELL      5.50220   5.65080   7.86560    90.049    89.975    90.007
ABSORB LESSTHAN       2.000

# Crystal Absorption Model
ABSORB MU      12.200
ABSORB MODEL XYZCORNER      4  3  4  0

ABSORB CORNER     -44.000    0.000   61.000
ABSORB CORNER      73.000    0.000   32.000
ABSORB CORNER     -69.000    0.000  -32.000
ABSORB CORNER      48.000    0.000  -60.000
ABSORB CORNER     -44.000   60.000   61.000
ABSORB CORNER      73.000   60.000   32.000
ABSORB CORNER     -69.000   60.000  -32.000
ABSORB CORNER      48.000   60.000  -60.000

# DAC Absorption Model
DAC TYPE   5
DAC OPEN        40.00       40.00
DAC GASKET       114.00  140.00    30.00  0.20
DAC ABSPSI CURVE         0.61
```

Absorption in DAC – key points

- **For corrections on a physical basis, the DAC, crystal and data must be described on a common reference system**
  - **Orientation matrix**
  - **Axial systems**
- **Keep things simple:**
  - **DAC face-on to beam at circles zero**
  - **Use hkl files with d-cosines**
- **Do inter-frame detector scaling afterwards**
- **Diamond dips and other outliers:**
  - **Identify in averaging or in refinement (Fo vs Fc)**

For previous users

- **Key changes to experiment (exp) files from Absorb 6:**
  - **Absorption coefficients now in mm-1**
  - **DAC component sizes in mm**
  - **New handling of negative intensities**
  - **New options to describe crystals in DACs**
  - **Distinction between DAC and phi-axis coordinate systems**