Indexing and Integration

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- Principles
 - What you need to do
- Practice
 - Relative merits of programs
 - Practical tuition and demonstrations



Intensity data collection



ECM Workshop Bergen, 2012

Synchrotron: correction for primary beam



- independent monitoring of the primary beam intensity
- measurement of standard reflections (point detector)
- integration software takes into account the primary beam intensity
 - information is fed into the program and used for scaling
 - information is obtained from the average intensities of the frames
 - information is obtained from the average intensities of the crystal



At synchrotrons....

- Also worry about the image/detector orientation!
 - Look at the frames...cell shadow and beamstop





D3 (HASYLAB) 4(3)-circle HUBER & MAR165 (CCD)

Pictures: Andrzej Grzechnik



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Peak hunting on area detectors

- Only hunt in allowed regions
 - Otherwise bg wrong
 - Spurious peaks found
- Software needs to handle DAC opening angle
- Even without Be seats, there are:
 - **Diamond spots (** λ and $\lambda/2$)
 - Gasket rings
 - Diffraction from pressure sensor
- Software needs to distinguish sample spots as far as possible



The DAC on the goniometer

It is strongly recommended that you always collect data with the DAC face-on to the beam when the diffractometer angles are at zero.



- □ If not, be very very very careful in defining:
 - The opening angle and DAC to the integration program



Noisy data

- **Typical laboratory DAC pattern**
 - Less collimation
 - Broader powder rings
 - Lower intensity of sample peaks
- Software also needs to define masks in 2theta
 - Also removes diamond doublediffraction
- Manually edit the peak list after search and before indexing
 - **Diamond spots (** λ and $\lambda/2$)





Data coverage

- Data coverage is limited
 - Nice to be able to see it!
- Indexing is more difficult
 - More sensitive to spots not from the sample
- **Software needs:**
 - Robust against mixed cr
 - Algorithms to handle '2d
 - Options for input of 'kno
- One approach:
 - Index → cell
 - If not what you want (e.g delete indexed peaks an



aks an limeispirate of data collected in air





Integration: area detectors

Software needs:

- Masking of blank areas of detector
- Masking of selected areas
- Background subtraction:
 global + local
- □ Nice things to have:
 - Automatic learnt profile
 - Multiple UB and rejection of overlaps





Integration: point detectors

- Accurate peak positions
 - Easy indexing
- Background
 - Mostly collimated out
 - Examine profiles to eliminate interference
- DAC restrictions
 - Only accessible data is collected
- More information on data collection and integration in the PD session



