

Experience with imgCIF at Diamond

Alun Ashton
(apologies Stuart Campbell)



How diamond got involved

- Liz Duke and Gwyndaf Evans
- 3 Phase 1 MX beamlines
- 3 ADSC Q315 detectors required to produce imgCIF/CBF
- 2 beamlines already in user mode third soon



Current status wrt CBF/imgCIF in MX

- Happy that there is no difference in the data between ADSC and CBF formats
- Mosflm known to process data – still awaiting that version mind you.
- Still awaiting a response from HKL2000
- Future MX detectors required to produce CBF
- 'unexpected' benefit of size

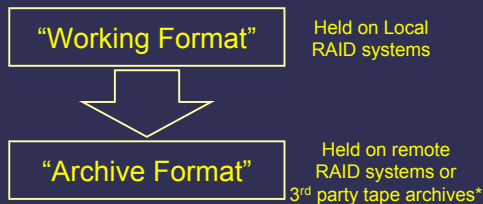


Why standardisation is important to DLS

- Data compatibility between beamlines.
- Support
- Long term storage and accessibility of data
- Potential UK policy that all data collected with the help of public funds is to be made available.



Diamond data strategy



Metadata will also be stored in a DB



Working Formats

- Variety of CCD formats
 - Photonic Science 4301 etc
 - ADSC 210,315
 - Oxford Diffraction Onyx, Ruby
 - Rigaku (Saturn 944 or 724) - possible
 - Mar 330
- Plain text / SRS format
- ImgCIF/CBF
- NeXus
- A variety of 'standard' image formats



Archive Format

- NeXus
- Ultimate aim is that other formats are incorporated into a NeXus file
- Short term aim is that if the working format is well defined then the NeXus file will reference the existing files.



imgCIF/CBF uptake as a working format on non MX beamlines

