Stable beam and good data – experience with beam (in–) stability at the SLS PX beamline X06SA

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Protein Crystallography



Time scales			
	period	importance	quality
SLS-run	weeks	medium	very good
User-run	~ day	medium	excellent
experiment	minutes	high	excellent
data frame	seconds	very high	very good
rocking curve	ms	highest	???











Absolute vertical beam position

Field strength of small gap undulators strongly depends on vertical position between magnets

Example: Bump scan in straight X06S with monchromator set to 12.311 keV

Gap [mm]	Vertical offset [µm]	E _{theo} [keV]
5.104	-425	12.260
5.142	-10	12.355



Multiple wavelength Anomalous Dispersion

Solution of the phase problem by making use of the anomalous scattering from more heavy atoms in the protein



Energy stability in MAD experiments

Typical relative core hole energy width: > 10⁻⁴
 Energy shift due to angular beam motion

$$\Delta E/E = \cot \Theta_B \cdot \Delta \Theta_B$$

Example: Se K-edge at 12.66 keV, Si (111) mono

-> cot⊖_B = 6.32

with $\Delta E / E < 10^{-5} \rightarrow \Delta \Theta_B < \pm 1.5 \mu rad$

Angular stability should be better than $\pm 1.5 \mu$ rad

Beam stability and data quality

Test system

high quality insulin crystals: mosaicity < 0.2 °
simultaneous movement of X11MA-ID1

Test variables

mode of SLS orbit feedback

- I flow speed of N2 crystal cooling system
- ø data collection time (and filtering)

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Data quality indicator internal R-factor

$$R(\text{int}) = \frac{\sum_{hkl} \sum_{i} |I_i(hkl) - \overline{I(hkl)}|}{\sum_{hkl} \overline{I(hkl)}}$$

Insulin crystal

Crystal size: 125 x 125 x 80 μm**3 Beam size: 15 x 5 μm**2











Conclusion

- The long term stability of SLS is great as long as the air condition works well
- The Slow-Orbit-Feedback is sufficient to stabilise the beam
- The effect of the Fast-Orbit-Feedback on data quality is most likely negative for very good crystals
- Sector External parameter like cryo-flow, sample mounting technology, etc. dominate data quality
- Slow residual drifts are effectively compensated by means of the beamline feedback system
- The long term goal is to use two XBPMs after the optics for feedback on the electron beam