11th International Workshop on X-ray Radiation Damage to Biological Samples - RD11



Contribution ID: 46

Type: Poster

Fixed target FEL crystallography for Phasing at 7.2 KeV

Fixed target sample holders for serial crystallography allow precise positioning of crystals into the X-ray interaction for optimization of the hit ray. In addition, they offer the possibility of collecting additional shots from the same crystal if the first X-ray pulse has not destroyed the crystal and for large crystals it allows the possibility of translating the crystal and collecting the data, which could be very useful for collecting redundant and isomorphic data. Apart from this, to test the potential of inverse beam for phasing serial crystallography data we collected data from cryocooled crystals of multiheme protein H1 at the LCLS beamline XPP, using a defocused beam (50 x 50 microns2) by carrying out the experiment at cryotemperatures we expected to extend the lifetime of the crystal enough to tolerate two 40 femtosecond exposures to each crystal at full beam intensity, as had already been demonstrated by Cohen et al (2014) for myoglobin crystals. Combining the first shot data would result in a practically radiation damage free data containing some anomalous differences. The second shot illuminates the same crystal volume and should yield a partially damaged data set. Combining both data sets would, on the one hand, increase the multiplicity of the anomalous measurements, while, on the other hand, degrading the anomalous signal. By analysing the data and the anomalous signal it should be possible to determine if merging of the two data sets is advantageous or detrimental.

References

Cohen AE et al. (2014) Proc Natl Acad Sci U S A Dec 2;111(48):17122-7

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