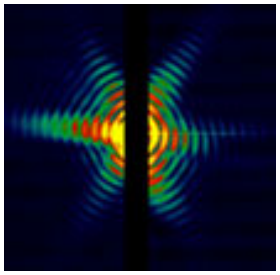

Contribution ID: **37** Type: **not specified**

Coherent Diffractive Imaging of Two and Three-Dimensional Membrane Protein Crystals using XFELs

Thursday 10 June 2010 17:30 (30 minutes)

The potential for imaging biomolecules using fourth generation XFEL sources is now being explored with the commisioning of beamline experiments having begun at the LCLS (Stanford). These experiments will employ the use of coherent X-ray diffractive imaging techniques by collecting snapshot diffraction patterns in a time regime that avoids nuclear damage in biomolecules. The opportunity to perform imaging of single biomolecules (such as membrane proteins) is present. Some membrane proteins form single two-dimensional crystals and submicron single three-dimensional crystals. Diffraction data collected from periodic samples (such as these small membrane protein crystals) will provide both an amplified intensity measurement and additional a priori constraints(the periodicity of the sample) that will benefit image reconstruction. We have simulated the diffractions produced using XFEL radiation for two-dimensional and three-dimensional submicron crystals of the membrane proteins lysozyme, potassium channels and bacteriorhodopsin for upcoming experiments. We seek to perform appropriate phase-retrieval on this data that will lead to high resolution solutions to membrane-protein structures.

Summary

Neutze et al. (1) first suggested the use of XFELs for biomolecular imaging since the timescale of X-ray pulses irradiating membrane-protein samples (~ 5-50 femtoseconds) is such that nuclear damage may be avoided. Further consideration has also been paid to damage to the electronic structure of such biomolecules under intense radiation (2).

Coherent Diffractive Imaging (CDI) is an imaging technique that has been developed to image objects that are non-crystalline (3)(4) with X-rays. The object structure is reconstructed from the diffraction data image using phase-retrieval algorithms (5)(6). It has been demonstrated that appropriate real-space constraints (information about the sample object such as its size) or implementation of knowledge about the wavefield in phase-retrieval algorithms improves the reconstruction of the sample (7)(8).

The collection of diffraction data and analysis from single molecules and small two-dimensional membrane protein crystals using XFEL pulses has been considered (9)(10)(11). We have performed diffraction simulations for submicron membrane protein crystals incorporating the X-ray intensities supplied at LCLS, Stanford. We seek to develop implement CDI techniques for resolving high resolution information from this data for experiments to be performed in the near future.

(1)Neutze et al., Nature, 2000
(2)Hau-Riege et al.,Phys Rev B., 2004
(3)Sayre, Acta Crystallographica, 1952
(4)Miao, Nature, 1999
(5)Gerchberg, Saxton, Optik, 1972
(6)Feinup, Applied Optics, 1978
(7)Nugent et al., Phys Rev Lett., 2003
(8)Quiney et al., Nature Physics, 2008

(9)Ourmazd et al., Nature Physics, 2009
(10)Spence, et al., Phys Rev Lett,2004
(11)Mancuso et al., Phys Rev Lett., 2009

Primary authors: Dr QUINEY, Harry (CXS University of Melbourne); Prof. NUGENT, Keith (CXS University of Melbourne); Ms RYAN, Rebecca (CXS University of Melbourne)

Presenters: Prof. NUGENT, Keith (CXS University of Melbourne); Ms RYAN, Rebecca (CXS University of Melbourne)