High Resolution 3-D X-Ray Diffraction Microscope

David Shapiro (dshapiro@xray1.physics.sunysb.edu), Janos Kirz, Chris Jacobsen(SUNY @ Stony Brook), John Miao(SSRL, Stanford University), Aaron Stein, David Sayre(SUNY @ Stony Brook)

When the diffraction pattern of an object is sampled on a scale finer than the Nyquist frequency, the diffraction pattern is oversampled. In theory, oversampling the diffraction pattern corresponds to surrounding the specimen with a no-density region [1]. When the no-density region is larger than the electron density region of the specimen the phase information is uniquely imbedded in the diffraction pattern and can be recovered by a Fienup type algorithm. Sampling the diffraction pattern on such a fine scale increases the risk of radiation damage to the specimen since more photons must be processed. It has been shown that biological specimens imaged with soft x-rays at liquid nitrogen temperatures can sustain a much higher radiation dose before morphological damage occurs[2]. In our current experiment, which is carried out at beamline X1B of the NSLS, a highly coherent beam of x-rays from the X1 undulator, illuminates a frozen hydrated yeast cell and the far field diffraction pattern is recorded on a backside illuminated CCD chip. The specimen, which has been plunge frozen in liquid ethane and is held to a copper TEM grid by several microns of vitreous ice, is maintained at liquid nitrogen temperatures throughout the experiment by mounting the grid on a cryo holder.

Ultimately, a full 3 dimensional diffraction data set will be obtained. To do this, we will make use of the Gatan ultra high tilt cryo holder. This holder is able to rotate the specimen around an axis perpendicular to the beam direction through a total angle of 160 degrees. The limited rotational motion of the holder results in a double wedge of data missing from the 3D diffraction cube. Computer simulations performed on a two dimensional model system, a 2D fake cell, suggest that the algorithm is able to reconstruct the missing intensities as well as the phases if the missing wedge is not too large.

References:

[1] J.Miao, J.Kirz, D.Sayre, Acta Crystallographica **D 56**, 1312-1315 (2000).

[2] J. Maser *et al.*, ``Soft x-ray microscopy with a cryo STXM: I. Instrumentation, imaging, and spectroscopy," *J. Microscopy* **197**, 68-79 (2000)