

High Resolution 3-D X-Ray Diffraction Microscope

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Abstract No.: Shap1159

Beamline(s): X1B

Introduction: The idea of applying the methods of x-ray crystallography to image non-crystalline materials has a long history^[1-4]. It was shown previously that this methodology could be used to image a micron sized non-crystalline specimen, consisting of micro-fabricated gold dots, to 65nm resolution^[5-6]. The current work attempts this with a micron sized biological specimen.

Methods and Materials: At beamline X1B, a highly coherent x-ray beam from the X1 undulator illuminates the specimen, a frozen hydrated yeast cell, and the far field diffraction pattern is recorded on a back-thinned CCD detector. In theory, oversampling the diffraction pattern of a finite specimen corresponds to surrounding the specimen with a no density region. The higher the oversampling the larger the no density region. When the no density region is larger than the electron density region of the specimen, the phase information is uniquely embedded inside the diffraction pattern. The oversampled diffraction pattern and a random initial phase are the input into a Fienup type algorithm, which attempts to reconstruct the phase information thereby allowing a direct calculation of the real space image. With this form of microscopy the resolution is only limited by the wavelength of the radiation and the angular extent of the recorded diffraction pattern instead of by optical elements.

Results: Recently, the first diffraction from a frozen hydrated specimen was recorded but these preliminary patterns were not complete so the effectiveness of the algorithm at reconstructing the real space image of a biological specimen could not be tested. Shown to the right are part of the recorded diffraction pattern and a low-resolution zone plate image of the scatterer, which is used for alignment. In future experiments we will record a complete 2-dimensional diffraction data set with which a reconstruction will be attempted and then the move towards 3-D data sets will be undertaken.

Acknowledgments: We would like to thank Steve Hulbert and Sue Wirick for their assistance.

References: [1] D. Sayre, "Prospects for long wavelength x-ray microscopy and diffraction," in *Imaging Processes and coherence in Physics*, edited by M. Schlenker (Berlin, 1980), pp. 229-235. [2] W.B. Yun, J. Kirz, D. Sayre, "Observation of the soft x-ray diffraction pattern of a single diatom," *Acta Crystallographica A* **43**, 131 (1987). [3] D. Sayre, "Note on "superlarge" structures and their phase problem," in *Direct Methods of Solving Crystal Structures*, edited by H. Schenk (New York, 1991), pp.353-356. [4] D. Sayre, H.N. Chapman, J. Miao, "On the extendibility of x-ray crystallography to non-crystals," *Acta Crystallographica A* **54**, 232-239 (1998). [5] J. Miao *et al*, "An extension of the methods of x-ray crystallography to allow imaging of micron-size non-crystalline specimens", *Nature* **400**, 342-344 (1999). [6] J. Miao, J. Kirz, D. Sayre, *Acta Crystallographica D* **56**, 1312-1315 (2000).

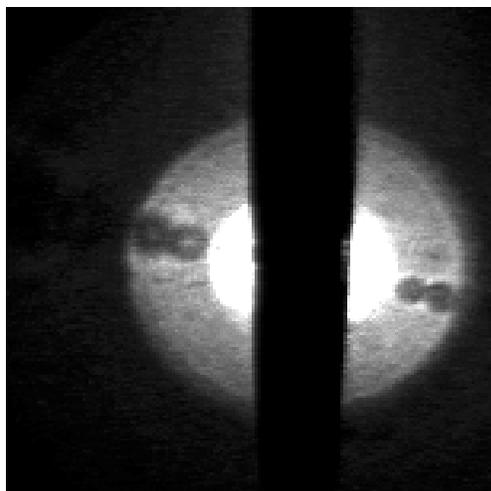


Figure 1. Low-resolution zone plate image used for specimen alignment. The dark central stripe is the beamstop and the bright central region is higher order contamination from the undulator.

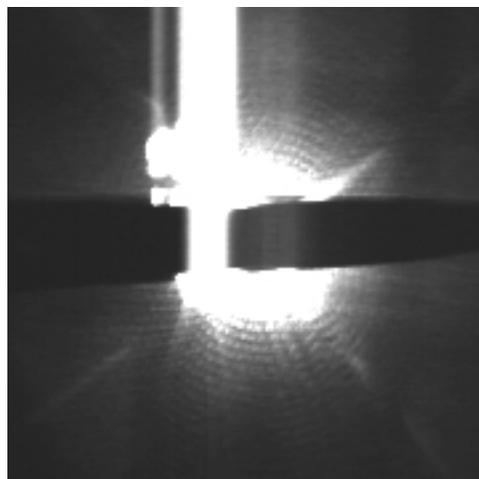


Figure 2. Section of a diffraction pattern from two frozen hydrated yeast cells. The black horizontal stripe is the beamstop and the bright vertical stripe is streaking due to CCD damage.