Acta Cryst. (2002). A58 (Supplement), C198

X-RAY SPECTROMICROSCOPY: HIGH RESOLUTION CHEMICAL STATE IMAGING IN COMPLEX ORGANIC SYSTEMS

<u>C. Jacobsen</u> T. Beetz M. Feser H. Fleckenstein B. Hornberger J. Kirz E. Lima M. Lu D. Shapiro A. Stein S. Wirick SUNY Stony Brook Dept. Physics & Astronomy Nicolls Road STONY BROOK NY 11794-3800 USA

Soft x-ray microscopy provides <50 nm spatial resolution imaging with an energy bandwidth of <0.2 eV for studies of complex organic systems. By acquiring a series of images across an absorption edge, a data set in three dimensions (X,Y, and energy) is obtained which exploits the chemical state sensitivity of x-ray absorption near-edge structure or XANES.

With known absorption spectra, maps of component concentrations can be obtained; with unknown spectra, multivariate statistical analysis methods can be used to understand the number and distribution of components and to find common spectra. Applications in biology and geochemistry are described. In addition, the status of experiments in diffraction and holographic imaging of frozen hydrated specimens will be described.

Keywords: X-RAY MICROSCOPY X-RAY SPECTROSCOPY XANES

Acta Cryst. (2002). A58 (Supplement), C198

ELECTRON PHASE MICROSCOPY TO OBSERVE VORTICES IN SUPERCONDUCTORS

A. Tonomura

Advanced Research Laboratory, Hitachi, Ltd. Hatoyama, Saitama, Japan ²SORST, Japan Science and Technology Corporation (JST), Tokyo, Japan ³Frontier Research System, The Institute of Chemical and Physical Research (RIKEN), Saitama, Japan

Bright beam sources, like lasers and synchrotron radiation, open new ways of investigating microscopic structures. In order to utilize the phase information of an electron beam for microscopy, we have continued to develop brighter electron beams since 1968. As it turned out, every time beam brightness was increased, new applications opened up. For example, the magnetic lines of force in h/e flux units can be observed as an electron interference micrograph [1]. In 1992, we dynamically observed [2] quantized vortices in superconductors by Lorentz microscopy using our 350-kV microscope. In Spring 2000, we completed a 1-MV microscope [3] that has the brightest beam ever obtained, and we have just begun obtaining various new results such as the observation of both vortices trapped along columnar defects in Bi-2212 film and a special arrangement of vortices, the chain-lattice state [5], reflecting the layered structure of the material. References

1) A. Tonomura et. al., Phys. Rev. Lett. 44 No. 21, 1430, (1980).

2) K. Harada et al., Nature 360, 51, (1992).

3) T. Kawasaki et al., Appl. Phys. Lett. 76, No. 9, 1342, (2000).

4) A. Tonomura et al., Nature 412, 620, (2001).

5) T. Matsuda et al., Science 294, 2136, (2001).

Keywords: LORENTZ MICROSCOPY, ELECTRON BEAM, SUPERCONDUCTOR

Acta Cryst. (2002). A58 (Supplement), C198

HIGH RESOLUTION 3-D X-RAY DIFFRACTION MICROSCOPY AND ITS POTENTIAL OF IMAGING SINGLE BIOMOLECULES J. Miao¹ T. Ishikawa² D. Sayre³ K. O. Hodgson⁴

¹Stanford Synchrotron Radiation Laboratory, Stanford Linear Accelerator Center, Stanford University, Stanford, CA 94309-0210, USA ²SPring-8/RIKEN, 1-1-1, Kouto, Mikazuki, Sayo-gun, Hyogo 679-5198, Japan. ³Department of Physics and Astronomy, State University of New York, Stony Brook, NY 11794, USA. ⁴Department of Chemistry and Stanford Synchrotron Radiation Laboratory, Stanford Linear Accelerator Center, Stanford University, Stanford, CA 94309-0210, USA

We report the development of a novel form of X-ray microscopy (see contribution by D. Sayre et al.) based on the coherent X-ray diffraction and the oversampling phasing method. By using coherent soft X-rays with a wavelength of 17 Å, the first demonstration experiment was carried out in 1999 to determine the 2-D structure of a non-crystalline specimen at 75 nm resolution. More recently, by using coherent X-rays with a wavelength of 2 Å from an undulator at SPring-8, the 2-D structure of a non-crystalline specimen at 7 nm resolution and a 2-D buried structure at 8 nm resolution have been experimentally determined. An algorithm was also developed for the reconstruction of 3-D images from a limited number of diffraction pattern projections without the need of interpolation. By employing this algorithm, for the first time the 3-D structure of a non-crystalline specimen at 55 nm resolution was reconstructed from a series of 2-D diffraction patterns. The 2-D and 3-D imaging resolution is currently limited by the exposure time and the computing power, while the ultimate resolution is limited by the X-ray wavelengths. We believe these results pave the way for the development of 3-D X-ray diffraction microscopy at atomic resolution, which can image thick specimens not accessible to scanning probe microscopy and transmission electron microscopy. In combination with the planned X-ray free electron lasers having ultra-short and extremely intense pulses, this form of X-ray microscopy could be applied to image single biomolecules at atomic or near atomic resolution. By using computer simulation, it has been shown that a molecular diffraction pattern at 2.5 Å resolution accumulated from multiple copies of single rubisco biomolecules each generated by a femtosecond-level X-FEL pulse can be successfully phased and transformed into an accurate electron density map comparable to that obtained by more conventional methods.

Keywords: OVERSAMPLING COHERENT X-RAYS, SINGLE MOLECULES

Acta Cryst. (2002). A58 (Supplement), C198

METHODS FOR PHASE RETRIEVAL IN THE INTERMEDIATE AND NEAR FIELD

<u>T.E. Gureyev</u>¹ A. Pogany¹ D.M. Paganin² S.C. Mayo¹ A.W. Stevenson¹ S.W. Wilkins¹

¹CSIRO Manufacturing Science and Technology Private Bag 33 CLAYTON SOUTH VICTORIA 3169 AUSTRALIA ²Monash University School of Physics and Materials Engineering

A number of different methods for optical phase retrieval are analyzed and tested using simulated and real X-ray images collected in the near and intermediate fields, i.e. in the regions where the Fresnel number is either much larger than or of the order of unity. As the extent of these regions is determined by the radiation wavelength and the size of the features being imaged, in a real experiment a single sample often has features of different size (resolution) that correspond to different imaging fields [1]. It has been demonstrated previously that in the near field the phase can be rapidly and accurately retrieved using one of the techniques based on the Transport of Intensity Equation [2]. Therefore, these techniques can be applied to low-resolution features of an image. The high-resolution components of the phase have to be reconstructed using alternative phase-retrieval techniques. The results presented are obtained using several techniques. These techniques allow phase retrieval from either a single in-line image collected in the near or intermediate field, or several images collected either at different defocus distances, or at a fixed distance, but with different radiation wavelengths. Applications of the techniques to visual improvement and quantitative analysis of in-line X-ray images collected in the near and intermediate fields are demonstrated. References

 Pogany, A., Gao, D. & Wilkins, S.W. (1997) Rev. Sci Instrum. 68, 2774-2782.
Nugent, K.A., Gureyev, T.E., Cookson, D.F., Paganin, D. & Barnea, Z. (1996). Phys.Rev.Lett. 77, 2961-2964.

Keywords: PHASE RETRIEVAL, X-RAY IMAGING, X-RAY HOLOGRAPHY