

both the intensity and the phase information and the three dimensional image of the object can be reconstructed. The most important limitation of this imaging technique is the spatial resolution, which is given by the wavelength and/or by the source size. In the last decade the introduction of soft x-ray instead of visible light tremendously improved the resolution which reached a few hundred angstrom [2]. An other line in holography, based on the inside source concept, was suggested recently [3]. We have applied this concept for the case of fluorescent x-rays emitted by a single crystal. We were the first to demonstrate theoretically [4] and experimentally [5] the feasibility of x-ray holography with atomic resolution. We have recorded the holograms of different crystals and successfully reconstructed the three dimensional order of the atoms.

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**PS15.01.16 RESONANT SCATTERING: TENSORS OF HIGHER RANK AND THETA DEPENDENCE.** David H. Templeton and Lieselotte K. Templeton, Department of Chemistry, University of California, Berkeley, CA 94720, USA

The resonant scattering of X rays by an atom is always anisotropic with respect to photon polarization and often changes with molecular orientation. The largest effects can be described by atomic tensors of second rank multiplied by polarization vectors for incident and scattered photons. When the finite size of the atomic wavefunctions cannot be neglected one must add tensors of higher rank with wave vectors as additional factors. A tensor of third rank is required to explain the scattering by some atoms in noncentrosymmetric sites (*Phys. Rev. B* **49**, 14850 (1994)). This term is proportional to  $\sin\theta$  and does not occur in absorption spectra. It changes sign on inversion with novel consequences on structure-factor algebra. Fourth-rank effects have been observed in both absorption and scattering (e.g. Dräger, et al., *Phys. Stat. Sol.* (b) **146**, 287 (1988); Finkelstein, et al., *Phys. Rev. Lett.* **69**, 1612 (1992)). They can be formulated as functions of the sum and difference of the wave vectors, proportional respectively to  $\cos 2\theta$  and  $\sin 2\theta$ . Only the first is observed in absorption spectra. The second-rank tensor term, as derived from perturbation theory, is independent of Bragg angle. Any change of resonant scattering with Bragg angle is contained in the higher terms, but the part which is isotropic for wave vectors can be treated as a change with theta of the second-rank parameters. The semiclassical model based on a continuum of anisotropic electric susceptibility can describe only some of these properties. We study the anisotropy of these tensors by measuring the changes of intensity with azimuth of weak or "forbidden" reflections chosen to be sensitive to one term or another. New experiments with pyrite at the Fe K edge will be reported.

**PS15.01.17 CONVERGENT BEAM MACROMOLECULAR CRYSTALLOGRAPHY USING POLYCAPILLARY X-RAY OPTICS.** J. B. Ullrich<sup>#</sup>, S. M. Owens<sup>\*</sup>, Q.-F. Xiao<sup>#</sup>, I. Yu. Ponomarev<sup>#</sup>, D. Carter<sup>+</sup>, R. C. Sisk<sup>+</sup>, and W. M. Gibson<sup>\*</sup>, <sup>\*</sup>Center for X-ray Optics, University at Albany, Albany, NY 12222 <sup>#</sup>X-Ray Optical Systems, 90 Fuller Rd., Albany, NY 12205, <sup>+</sup>Laboratory for Structural Biology, NASA Marshall Space Flight Center, Huntsville, AL 35812

The viability of macromolecular crystallography is dependent on the ability to view large volumes of reciprocal space during a

single x-ray exposure. The most popular methods used to do this are precession, rotation (or oscillation), and Laue photography, but a convergent beam can, in principle, achieve the same result. Although the convergent beam technique has been considered as an alternative to the oscillation method (Wyckoff and Agard, *The Rotation Method in Crystallography*), it has not been generally adopted by the crystallographic community. Polycapillary x-ray optics can collect x-rays over large solid angles and re-focus the x-ray beam to < 1 mm spots, yielding significant intensity gains at the crystal, and simultaneously exposing large volumes of reciprocal space without having to oscillate the crystal. The ability to generate convergent beams with existing sources, coupled with the potentially large intensity gains, warrants serious re-examination of the convergent beam method. This technique could be particularly important for the case of small crystals, since focal spot sizes of 20 - 40 microns are obtainable with strong focusing. We have conducted a study of convergent beam crystallography using polycapillary x-ray optics and its effect on data collection and quality. The results of this study, including the potential for significantly faster data collection with smaller crystals, will be presented.

**PS15.01.18 TRAVERSE PATTERN OF DEFECTS IN THE BRAGG CASE.** T.S. Urugami, H. Kobayashi and D. Orii, Faculty of Engineering, Okayama University of Science, Okayama, 700 Japan

On the camera with traverse mechanism for X-ray diffraction with an incident wave of finite width, the defects in a Silicon single crystal was observed in the Bragg case by using the diffracted wave which comes out from the inner part of a crystal. The diffracted wave can be observed without disturbance from the directly reflected wave when the width of the incident wave is adjusted as to eliminate the overlapping of the directly reflected wave and the image-forming one at the exit point. The Pendelloesung fringes in the Bragg case are strong in the inner part of the specimen, but fade out on approaching the entrance surface except at the incident point and around its neighbourhood. A strong wave is produced by a defect in a region where the Pendelloesung fringes are intense, and a faint wave is produced in a region where those are weak.

The experiment was done with an X-ray source, entrance slit, specimen crystal, receiving slit and plate. The leaf of one side of the receiving slit was used to stop the beam of direct reflection by 220 and 440 net planes in a Silicon single crystal. The plate receives the crystal wave coming out from the surface except the incident point since the beam of direct reflection is stopped by the receiving slit. As the entrance slit is narrow, the width of transmitted wave traveling in the crystal is not wide. The non-diffracted component of the diffracted wave may have the same width as the entrance slit. The kinematical images of defects are produced from the transmitted wave in the region where the non-diffracted component flows.

The background is mainly increased by the crystal misorientation during the traverse motion and by the Compton inelastic scattering. The Compton scattering may be reduced by making a non-diffracted component narrower. The entrance slit of 10Å m width and the narrower turned out to have been effective for this purpose.