a collimating optic with a linear capture angle of 0.15 rad, 12.5μm channel size, and output area of 3.1 cm was placed into a standard Bragg-Bretano diffractometer. Capillary optics provide even larger signal gains for very small samples. More than an order of magnitude signal increase was achieved for a 0.3 mm Lysosyme crystal by employing an optic with a 0.1 rad capture angle and 5 mm output diameter. This paper will present a review of the broad range of applications of capillary optics to diffraction systems.

PS15.01.12 ON THE X-RAY DIFFRACTION BY PERFECT ABSORBING CRYSTALS. Alfonso E. Merlini, 21027 Ispra (Va), Italy

Previous measurements of the (111) intensities diffracted by a perfect Ge crystal in the Bragg case, at frequencies of the incident radiation close to the K absorption edge, were considerably higher than those calculated by the dynamical theory of X-ray diffraction[1]. The theory was modified so that the Kramers-Kronig dispersion relations be satisfied for each value of the glancing angle of the incident beam. In this way the photoelectric absorption contribution f'_{dyn} to the real part of the form factor depends on the glancing angle as the imaginary part does. f'_{dyn} is equal to the product of the intensity of the internal wavefield at the absorbing K-electrons by the contribution f'_{at} predicted by the anomalous dispersion theory of the individual atom (for simplicity the effects of the crystal field on the matrix elements of the absorption transition are neglected). The corresponding Darwin-Prins curves are higher than those foreseen by the present form of the dynamical theory of absorbing crystals and the integrated intensities are 20-30% greater. For example the relative calculated integrated intensities of the (111) Bragg reflection by a thick Ge crystal for a frequency of the incident beam 7.64 eV higher than the frequency of the absorption edge are about 1.58, 1.44 and 1.12 by taking the absorption contributions to the real part of the form factor equal to 0, f'_{dyn} and f'_{at} respectively. The dynamical theory in its present form is a good approximation if the absorption contribution to the real part of the form factor is much smaller than its basic part. It is proposed that this theory be modified to take into proper account the dispersion relations. An important conclusion is that $f'_{dyn} \approx 0$ (the effect of the anomalous dispersion is wiped out) in that part of the interference region where the absorption is small. Since the internal wavefield depends on the absorption contribution to the real part of the form factor, a consistent value of this contribution can be obtained either by a numerical solution of the equation of f'_{dyn} or by an iteration procedure(applicable for incident frequencies a few eV away from the absorption edge) of the same equation. A comparison with the above mentioned experimental results is satisfactory. The proposed modified theory can be readily extended to the Laue case, to different absorption phenomena and to the diffraction of other types of radiation by perfect crystals.

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PS15.01.13 OBSERVATION OF PHASE CHANGE OF X-RAY POLARIZABILITY BY THE ROCKING CURVES IN THE BRAGG CASE. R. Negishi, T. Fukamachi, S. M. Zhou, Z. C. Xu, M. Yoshizawa, I. Matsumoto[1)], T. Sakamaki[2)], T. Kawamura[3)], T. Nakajima[4)], Saitama Institute of Technology, Okabe, Saitama 369-02,Japan, University of Library and Information Science, Tsukuba, Ibaraki 305, Japan, [2)]JEOL LTD, Akishima, Tokyo 196, Japan, [3)]Yamanashi University,Kofu, Yamanashi 400, Japan, [4)]Photon Factory, KKK, Oho, Tsukuba, Ibaraki, 305, Japan

Rocking curves of the transmitted beam for GaAs 600 diffraction in the symmetric Bragg case were measured just below the K-absorption edge of Ga by using X-rays from synchrotron radiation. When X-ray energy is 9eV below Ga K-absorption edge, the rocking curve shows the asymmetry: the intensity in the lower angle region of the exact Bragg angle is larger than that in the higher angle region. The reversed asymmetry is observed in the rocking curve at 3eV below Ga K-edge, i.e. intensity in the higher angle region is larger than that in the lower angle region. The critical energy of this reversal is about 6eV below Ga K-edge.

Based on a dynamical theory of X-ray diffraction with absorption effect taken into account[1)], the diffracted and the transmitted intensities were calculated. By comparing the measured rocking curves with the calculated ones, it is elucidated that the asymmetry of the transmitted rocking curves described above depends on the value of the phase difference δ, which is the difference of phase factors of the Fourier transforms of the real and the imaginary components of the X-ray polarizability. The phase difference δ is a function of crystal structure as well as anomalous scattering factor. Similar asymmetric rocking curves in the Laue case have been reported by Fukamachi et al.[2)]. It is pointed out that this change of the asymmetry is potentially useful in the phase determination of the structure factors.

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2) T. Fukamachi, R. Negishi, S. M. Zhou, M. Yoshizawa, T. Sakamaki, T.Kawamura, T. Nakajima, Acta Cryst.(1996), in press.

PS15.01.14 POLYCAPILLARY X-RAY OPTICS FOR MACROMOLECULAR CRYSTALLOGRAPHY. S. M. Owens*, J. B. Ullrich#, I. Yu. Ponomarev#, Q.-F. Xiao#, D. Carter+, R. C. Sisk+, and W. M. Gibson*. *Center for X-ray Optics, University at Albany, Albany, NY 12222; #X-Ray Optical Systems, 90 Fuller Rd., Albany, NY 12205; +Laboratory for Structural Biology, NASA Marshall Space Flight Center, Huntsville, AL 35812.

Polycapillary x-ray optics have shown great potential in macromolecular x-ray crystallography. Incorporation of polycapillary x-ray optics into existing x-ray sources yields significant increases in beam intensity compared to simple collimation. The optic used in this work collects x-rays from the source over a large solid angle (6° capture angle) and redirects them into a quasi-parallel beam (<0.2° divergence) of 5 mm diameter. Using this optic coupled to a modified RU200 rotating anode source, we recently produced a gain in flux through a 0.3 mm collimator of more than an order of magnitude over a comparable graphite monochromated source. Using large, microgravity grown lysozyme crystals as a "standard", we collected full data sets with and without Ni filtering of the primary beam (the high energy rejection of the optics allows measurements to be done without further filtering). Without filtering, a complete data set, to a minimum of 1.54 Å resolution, was obtained within 13.4 hours with a final Rmerg of 7.29 % (based on all observations). The data were collected with a Siemens Multiwire detector, read by FRAMBO and analyzed using SAINT. We have made similar measurements with a prototype optic which produces a weakly convergent beam (< 1° convergence), and further increases the flux gain to more than 100. Full data sets using this optic have also been collected. Details of the data reduction and analyses, as well as applications to structure determinations, will be presented.

PS15.01.15 X-RAY HOLOGRAPHY WITH ATOMIC RESOLUTION Miklós Tegze and Gyula Faigel, Research Institute for Solid State Physics, H-1525 Budapest, P.O.Box 49, Hungary.

One of the basic problems in crystallography is that in the conventional diffraction experiments only the intensity of the scattered radiation is recorded, its phase is lost. In holography [1], the scattered radiation is mixed with a reference wave and the resulting interference pattern is recorded. The hologram contains 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#, S. M. Owens*, Q.-F. Xiao#, I. Yu. Ponomarev#, D. Carter+, R. C. Sisk+, and W. M. Gibson*, *Center for X-ray Optics, University at Albany, Albany, NY 12222 #X-Ray Optical Systems, 90 Fuller Rd., Albany, NY 12205, +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. Uragami, 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 directy 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 narower turned out to have been effective for this purpose.