15.X-1 FOLLOWING MOLIÉRE'S THEORY WITH SYNCHROTRON RADIATION. By N. Kato, Department of Physics, Faculty of Science and Engineering, Meijo University, Nagoya, Japan.

This paper is nothing new but intends to serve the role of a traffic policeman on the street called "crystal optics" which was well paved by P. P. Ewald and G. Moliére. In the conventional diffraction theory, we start with the relation

$$4\pi \underset{\sim}{P}(\underset{\sim}{r}) = \underset{\sim}{\chi}(\underset{\sim}{r})\underset{\sim}{E}(\underset{\sim}{r}) \qquad (1)$$

where $\underset{\sim}{P}$ and $\underset{\sim}{E}$ are electric polarization and electric vector respectively at a position $\underset{\sim}{r}$ in crystals. This implies that the polarizability $\underset{\sim}{\chi}$ is "local and scalar". Ewald started his theory (1916, 1917) with a tensor $\underset{\sim}{\chi}$, and Moliére, by a quantum mechanical treatment, recognized it non-local in the sense

$$4\pi \underset{\sim}{P}(\underset{\sim}{r}) = \int_c \underset{\sim}{\chi}(\underset{\sim}{r},\underset{\sim}{\xi})\underset{\sim}{E}(\underset{\sim}{\xi})d\underset{\sim}{\xi} \qquad (2)$$

where the integral domain c covers the whole crystal. Of cource, the correction term for χ is extremely small unless the overlapping of wave functions of neighbouring atoms is appreciable or the wavelength is close to the absorption edge. After SR or high intensity X-ray sources become available, it is a challenge to detect the effect, since it reflects direct informations on bonding natures of solids. Reminding the spatial periodicity of $\underset{\sim}{\chi}$ with respect to both $\underset{\sim}{r}$ and $\underset{\sim}{\xi}$, one can write down dynamical equations in the Fourier space as

$$(\underset{\sim}{K}^2-\underset{\sim}{K}_g^2)\underset{\sim}{d}_g = \textstyle\sum_h [\underset{\sim}{k}_g \times [\underset{\sim}{k}_g \times \underset{\sim}{\chi}_{g,h}\cdot\underset{\sim}{d}_h]] \qquad (3)$$

where the notations are those in the standard dynamical theory except that

$$\underset{\sim}{\chi}_{g,h} = \chi_{g-h} + \Delta\underset{\sim}{\chi}_{g,h} \qquad (4)$$

and $\Delta\underset{\sim}{\chi}_{g,h}$ is the double Fourier transform of $\Delta\underset{\sim}{\chi}(\underset{\sim}{r},\underset{\sim}{\xi})$. Some remarks are described in order.

(1) One beam case; only $\underset{\sim}{d}_o \neq 0$: The optical activity (rotation of polarization) is expected exactly in the same manner as the ordinary crystal optics. Difficulties in the experiment lie not only in the smallness of $\Delta\underset{\sim}{\chi}_{0,0}$ but in harmful simultaneous reflections. (M. Hart and A. Rodriguess, 1981, Phil. Mag. B43, 321.) Nevertheless, apparently, $\Delta\underset{\sim}{\chi}_{0,0}$ exists.

(2) Dichroism is also expected due to the imaginary part of $\Delta\underset{\sim}{\chi}_{0,0}$. E. Stern et al. (Phys. Rev. Letters, 1976, 37, 298) and D. H. and L. K. Templeton (Acta Cryst. A, 1980, 36, 237) have already observed it in EXAF's regions. It is desirable to experiment under the guarantee of no Bragg reflection.

(3) The kinematical case; $\underset{\sim}{d}_g \neq 0$ but small: Anisotropic scatterings were observed by D. H. and L. K. Templeton (Acta Cryst. A, 1982, 38, 62; ibid. 1985, 41, 133). The formal theory relating to the extinction rule is given by V. E. Dmitrienko (Acta Cryst. A, 1984, 40, 89 and others).

(4) The dynamical case: $\underset{\sim}{d}_o \sim \underset{\sim}{d}_g$: It seems that the difficulty lies in the art of crystal growth. Perfect crystals having strong anisotropicity in a molecular level are required as specimens.

15.X-2 X-RAY BIREFRINGENCE, ANOMALOUS SCATTERING, AND THE PHASE PROBLEM. David H. Templeton and Lieselotte K. Templeton, Department of Chemistry, University of California, Berkeley, CA 94720, USA.

With linearly-polarized synchrotron radiation we have observed strong birefringence near absorption edges for several substances as dichroism or pleochroism in absorption spectra and as anomalous scattering which requires description by a complex tensor rather than a complex scalar (Templeton & Templeton, Acta Cryst., 1980, A36, 237-41; 1982, A38, 62-67; 1985, A41, 133-42, 365-71). The three principal values and the orientation of this tensor for Se in tetragonal (anhydrous) selenolanthionine have been measured by least-squares refinement somewhat like that for anisotropic thermal motion, but with polarization vectors replacing the h vector in the expression. Reflections forbidden by a screw-axis rule are observed in sodium bromate near the Br K absorption edge and vary with azimuthal angle according to theory (Templeton & Templeton, Acta Cryst., 1986, A42, 478-81; Dmitrienko, Acta Cryst., 1984, A40, 89-95). This variation for 00ℓ permits direct observation of the magnitude and phase of the bromine-only part of the structure factor of 0,0,2ℓ, an allowed reflection. This technique is a method of selective diffraction in which atoms of a single element contribute to the signal, and it can reveal their positions with precision. For general reflections the manipulation of intensity by a change of orientation with respect to polarization can be used to determine structure-factor phases in the same ways as in multiple-wavelength methods. Research was supported by NSF Grant CHE-8515298 using facilities at Stanford Synchrotron Radiation Laboratory supported by DOE and NIH and at Lawrence Berkeley Laboratory supported by DOE.

15.X-3 POLYCRYSTALLINE DIFFRACTION AND SYNCHROTRON RADIATION. By W Parrish, IBM Almaden Research Centre, San Jose, California 95120, and M Hart, Department of Physics, The University, Manchester M13 9PL

During the last three years at Stanford we have developed parallel beam x-ray geometries for powder diffraction. With a 111 channel cut silicon monochromator matched to standard sample geometries and no post specimen monochromator we achieve high resolution, perfectly symmetric peak profiles and obtain the opportunity to measure diffraction patterns in either detector angle scanning (2θ) mode or in energy dispersive (E) mode. Since there are no constraints on sample geometry when parallel x-ray beams are used, a number of diffraction techniques, which are difficult or impossible to exploit with conventional focussing diffractometers, become routine. Samples can be studied in both reflection and transmission geometry in the same apparatus.

In essence we use the high intensity white radiation in five ways: High intensity is essential for studies of thin films or surfaces but the high intensity is also used with perfect crystal monochromators to provide a perfectly symmetric instrument function. The spectral range is used to match sensitivity to the problem in hand, to exploit anomalous dispersion phenomena and to operate in high resolution energy dispersive mode.

Profile analysis based upon a high intensity narrow instrument function becomes a very powerful experimental method of analysis. By working at a short x-ray wavelength we have been able to perform the first three dimensional analysis of particle size, morphology and strain in palladium powders.

Texture studies in very thin films which have a very high degree of preferred orientation are not possible

with the necessary sensitivity using conventional methods. By energy dispersive diffraction we have been able to determine preferred orientation parameters in thin palladium films grown in (111) orientation and co-deposited with rare gases.

Structure analysis as a function of depth in thin films and surface layers is an exceptionally important problem in various technologies. X-ray penetration can be limited by glancing incidence to a few tens of Angström units while the high intensity still allows 2θ-scans to be made in a reasonable time. Control of fluorescence and signal-to-background is important and it is achieved by a suitable choice of wavelength. Quantitative measurements of composition against depth have been made in thin layers of material in the Fe_3O_4 - Fe_2O_3 system.

15.X-5 BRAGG REFLECTION X-RAY OPTICS FOR SYNCHROTRON RADIATION SOURCES. By M Hart, Department of Physics, University of Manchester, Manchester, M13 9PL

Bragg reflecting perfect crystals are well matched to the characteristics of present day synchrotron radiation sources. By comparison with advances foreseen in the development of insertion devices to produce very high brightness sources on the next generation of storage rings, consideration of the next generation of x-ray optical beamlines is still at the prehistoric stage. There is an international obsession with the problems caused by beam-heating which, while important, is secondary to the problems which arise in x-ray optical design. For many situations, where the high source brightness must be delivered at the specimen position with good signal-to-background, almost no suitable x-ray optical systems exist even as coneceptual designs.

During recent years perfect silicon crystals and the appropriate dynamical diffraction theory have been exploited in the invention of almost all of the necessary x-ray optical components. Thus, background free monochromators and collimators for spectroscopy and small angle scattering, harmonic-free spectrometers, tunable polarizers and analysers, quarter wave plates, variable resolution crystals spectrometers, phase and amplitude modulators and x-ray interferometers have all been demonstrated. Of these only low-harmonic spectrometers have so far been implemented on a routine basis. Other x-ray optical systems have been used by specialist groups; some results will be reviewed.

15.X-4 ULTRA SAS WITH POINT FOCUSING GEOMETRY USING SYNCHROTRON RADIATION. By U.Bonse, R. Pahl and R. Nußhardt, Institute for Physics, University of Dortmund, Postfach 50 0500, 46 Dortmund 50, and HASYLAB/DESY, Hamburg, Fed. Republic of Germany.

Most high resolution small angle scattering cameras employ the so-called infinite slit height geometry, i.e. the measured pattern does not directly represent the original 2D-scattering pattern of a given sample but only a vertically integrated modification of it. In order to retrieve the richer information contained in the 2D-pattern more or less labourious and occasionally quite dubious desmearing procedures have to be applied to the measured data. Such methods fail in particular when the sample and hence also the original scattering pattern is lacking rotational symmetry about the incident beam. However, as will be shown here, a SAS camera featuring point geometry, momentum resolution at the level of 10^{-5} reciprocal angstroms and, at the same time, reasonable intensity can be realized by combining outstanding properties of SR, namely its excellent collimation and high brightness, with the use of multiply reflecting groove crystals in two diffraction planes at right angle to each other (Bonse and Hart, ZS Physik 189 (1965),151). Because SR is already sufficiently collimated in the horizontal plane, no groove crystal diffracting in that plane is needed in front of the sample, which is in contrast to the situation encountered at the conventional x-ray tube where crystals diffracting in either plane are necessary behind and before the specimen. First results obtained with test samples will be presented.

15.1-1 MICROCRYSTAL DIFFRACTION TECHNIQUES. By J.M. Newsam and H.E. King, Jr., Exxon Research and Engineering Company, Route 22 East, Annandale, NJ 08801, U.S.A.

Exploitation of the brightness of synchrotron X-radiation in diffraction experiments on microcrystals in the 1-15μm size range has required the development of techniques additional to those employed in conventional single-crystal X-ray diffraction. Workable methods for microcrystal selection and mounting, diffractometer alignment, background reduction, microcrystal orientation matrix definition and optimization, and intensity data collection and reduction are described. These techniques enable near-routine collection of intensity data sets from microcrystals $\geq$5μm, and perhaps smaller. Data for a selection of materials with known structures have been collected on beamline X10A at the National Synchrotron Light Source, Brookhaven. Results are summarized and considerations associated with analyses of unknown structures are also addressed.