Ewald Medal Lecture

A PERSONAL HISTORY OF DYNAMICAL DIFFRACTION THEORY by Norio Kato*, Department of Physics, Faculty of Science and Technology, Meijo University, Nagoya, Japan

As introduction, the essence of the Ewald dynamical theory will be reviewed briefly. The theory amounts to the microscopic foundation of X-ray optics in perfect crystals. It predicts a characteristic line profile of the Bragg reflection and interference (Peedelluseng) singulars, which were experimentally confirmed much later. The theory was completed as early as 1917. In his mind, it was a natural extension of his fundamental theory of crystal optics for any wavelength by X-rays. Astonishingly, this theory was his doctoral thesis finished in 1912 before Land's discovery of X-ray diffraction.

Next, the present author would like to mention why he has become interested in dynamical diffraction phenomena. It will be followed by a few theoretical developments carried out under encouragements and guidances of Professor Paul Ewald. Finally, a statistical dynamical theory will be explained because the author is interested in at present. This approach intends to give a sound base for understanding extensive phenomena, which is a long-lasting problem in crystallography, and to give a theoretical tool for characterizing crystal perfection of nearly perfect crystals like Si.

Main Lectures

ML-01.01 3RD GENERATION X-RAY SYNCHROTRON: FIRST EXPERIMENTS FROM ESRF TROIKA BEAM LINE by J. Ala-Nieslet*, C. Grubel, J. P. Legrand and M. S. Lehmann, Exp. Div., ESRF, BP 220-38043 Grenoble, France

Commissioning of a synchrotron beam line is done best by carrying out some typical, real experiments. Here we describe some experiments at the open beam line TROIKA at ESRF. The source is an 1.6m long undulator (period 46mm) with variable gap and taper, situated in a high beta-section of the storage ring. The source size and beam divergence parameters (FWHM) are 430 μrad (horizontal) and 0.2mm 16 μrad (vertical). At the minimum gap of 20mm the energy of the third harmonic is 7keV, raising to 12keV at a gap of 26.7mm. Experimental spectra, i.e. number of photons/sec./0.1% bandwidth through a pinhole, were measured with different monochromator crystals and found to be in excellent agreement with calculations, both with respect to shape and absolute flux. We report on experiments illustrating the variety of research that can be carried out at the TROIKA beam line:

(i) Protein crystallography using an image plate detector and the 5th harmonic energy 14.95keV of the undulator. An example is Seryl-β-hexapeptide Thermus thermophilus co-crystallized with D-β-(N- L-erythro-sulfamoyl) adenosine (with S. Chustak et al., EMBL). Another is a MAD study of a dodecyl of N-Cadherin (with W. Hendrickson, Columbia University, N.Y. and A. Thomson, EMBL with calcium replaced by Yb having an L3 absorption edge at 8.948keV in the 3rd harmonic in the undulator spectrum.

(ii) Packing of amphiphilic molecules (C16H33COOH) in a monolayer on a liquid substrate in particular melting of short-chain acids (C8, C9, 16, 12, 14) over water with B. Borje et al., Univ. Grenoble) and phases of the long chain acid with n=29 over mixtures of water and formamide subphase (with Heiserowitz et al., Wexlermann Institute) were studied. Here we used grazing incidence diffraction geometry in a Langmuir trough and a nitrogen position-sensitive detector behind a Soller collimator.

(iii) Magnetic scattering from the spiral phase in Holmium with polarized analysis carried out on several L-edge resonant energies (with B. Gicke, NSLS Brookhaven, J. Boyer et al., Riso and C. Vettier). ESRF were investigated.

(iv) Diffraction from thin, amorphous diamond-like films of carbon (with R. Perdanbann et al., Riso). In addition the beam line has been used to test different schemes for monochromator crystal cooling (Freund et al., ESRF) and for preliminary experiments on nuclear resonance scattering (Ruffer et al., ESRF)

ML-01.02 MICROCTOMOGRAHY, by U. Bonsa, Phys. Department, University of Fortmth, Germany

With increasing availability of highly collimated and intense synchrotron x-radiation generated by dedicated storage-rings of the third generation, absorption microtomography μCT has developed to higher spatial resolution and enhanced ability to distinguish between different elements or even different binding states of the same element. Furthermore, the employment of SSD detectors combined with perfect-crystal x-ray optical magnifiers made it possible to attain 1 to 2 μm resolution at still reasonable measuring speed. For instance, if we consider a 'good contrast' sample, then at an optimized source like the ESRF, in order to image a 4 mm sample volume at 2μm μm voxel volume, a measuring time of the order of one hour would be required. In other words, a one-hour measurement (followed by some computation time) yields the precise knowledge of the absorption 'density' at some 6x103 sample locations, representing a huge amount of structural information.

μCT is used to image in three dimensions and nondestructively to details of samples of all kinds, mainly in Materials Science, Biology, and Medicine. In the latter field the study of bone structure and its change with the development of various bone diseases appears to be very promising. The three-dimensional nature of structural μCT data is in principle superior to the two-dimensional information which is conventionally obtained from the light/microscopy inspection of histological sections, provided comparable spatial resolution can be achieved with μCT, which is now almost the case. Other applications presented will include 3D-images of alloy phases in light metals and the investigation of fiber distribution and dynamics in composite materials.

The state of the art of μCT and further possible developments will be described.