

Main Lectures

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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 (Pendellosung) fringes, 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 to X-rays. Astonishingly, this theory was his doctor thesis finished in 1912 before Laue'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 extinction 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 SYNCHROTRONS-FIRST EXPERIMENTS FROM ESRF TROIKA BEAM LINE by J. Als-Nielsen*, G. Grubel, J.F. LeGrand and M.S. Lehmann, Exp. Div., ESRF-BP220-F38043 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 1mm, 35 μ rad (horizontal) and 0.2mm, 16 μ rad (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 calculation, 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-tRNA synthetase *Thermus thermophilus* co-crystallized with 5-O-(N-(L-seryl)-sulfamoyl) adenosine (with S. Chusack et

al., EMBL). Another is a MAD study of a double dimer of N-Cadherin (with W. Hendrickson et al. Columbia University, N.Y. and A. Thomson, EMBL) with calcium replaced by Yb having an L_{III} -absorption edge at 8.948keV or the 3rd harmonic in the undulator spectrum.

(ii) Packing of amphiphilic molecules ($C_nH_{2n+1}COOH$) in a monolayer on a liquid substrate, in particular melting of short-chain acids (n=8, 9, 10, 12, 14) over water (with B. Berge et al, Univ. Grenoble) and phases of the long chain acid with n=29 over mixtures of water and formamide subphase (with Leiserowitz et al, Weizmann Institute) were studied. Here we used grazing incidence diffraction geometry in a Langmuir trough and a linear position-sensitive detector behind a Soller collimator.

(iii) Magnetic scattering from the spiral phase in Holmium with polarization analysis carried out several L-edge resonant energies (with D. Gibbs, NSLS Brookhaven, J. Bohr et al., Riso and C. Vettier, ESRF) were investigated.

(iv) Diffraction from thin, amorphous diamond-like films of carbon (with R. Feidenhansl 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 MICROTOMOGRAPHY. By U. Bonse*, Physics Department, University of Dortmund, Germany.

With increasing availability of highly collimated and intense synchrotron x-radiation generated by dedicated storage-ring sources of the third generation, absorption microtomography (μ CT) 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 CCD detectors combined with perfect-crystal x-ray optical magnifiers made it possible to attain 1 to 2 μ m 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 $\frac{1}{2}$ mm³ of sample volume at $2 \times 2 \times 2$ μ m³ 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 6×10^7 sample locations, representing a huge amount of structural information.

μ CT is used to image in three dimensions and non-destructively structural details of samples of all kinds, mainly in Materials Science, Biology, and Medicine. In the latter field the investigation of bone structure and its change with the development of various bone diseases appears to be very promising. The three-dimensional nature of structural μ CT data is in principle superior to the two-dimensional information which is conventionally obtained from the lightmicroscopical inspection of histological sections, provided comparable spatial resolution can be achieved with μ CT, 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 μ CT and further possible developments will be described.