to enable us to commence the structural analysis by the molecular replacement method. In addition, we have collected data from BEV and HRV2 crystals with anti-viral drug bound (WIN compounds), an HRV2 monoclonal antibody escape mutant, and a possible HRV2-FV antibody fragment complex. We will report the stage of data processing and discuss problems imposed by large cell dimensions.

PS-01.02.07 A NEW MACROMOLECULAR CRYSTALLOGRAPHY STATION ON THE BEAMLINQ BL-18 AT THE PHOTON FACTORY. By N. Watanabe1, S. Aida1, A. Nakagawa1,2, and N. Sakabe1,1 Photon Factory, National Laboratory for High Energy Physics, Tsukuba, Ibaraki 305, 1) The Institute of Physical and Chemical Research (RIKEN), Wako, Saitama 351-01, JAPAN.

A new experimental station (BL-18B) has been constructed on the bending-magnet beamline at the Photon Factory (PF) to extend its capability for macromolecular crystallography. The branch beamline is equipped with a 3m long fused silica bend cylinder mirror with 1:1 focusing, located 13.7m from the source. The surface of the focusing mirror is cylindrically polished and platinum coated with a sagittal radius of 413mm, and bent to a radius of ca. 450mm. The glancing angle of the X-ray beam with the mirror is set to about 3mrad, which gives a cut-off wavelength of approximately 0.4A. The mirror can focus the X-ray beam to about 0.04mm (vertical) x 1.2mm (horizontal), which is consistent with the expected size simulated by the raytracing technique. The monochromator is a fixed-exit double-crystal, located 23.1m from the source. The monochromator consists of two kinds of flat crystals, usually silicon (111) and germanium (111), mounted parallel on the goniometer. The two types of crystal are therefore interchangeable without opening the vacuum chamber. The monochromator T0 range is 5° to 70°. Photon flux of the monochromatic beam is 9.6 x 10^9 Photons/sec (Si) and 2.3 x 10^10 Photons/sec (Ge) at 1.38A at the sample position when the PF ring is operated at 2.5GeV, 300mA and the acceptance of the first slits is 0.2mrad (vertical) and 2.0mrad (horizontal).

BL-18B has been built as an end station in order to have enough space available for installing a large camera and other instruments in the experimental hutch. The station will extend the capability at PF beyond what is provided for with the Weissenberg camera (Sakabe, N., NIM,1991, A303, 448) at the BL-6A2 station (Sato, Y. et al., Rev. Sci. Instrum., 1989, 60, 2394). In addition to increasing the experimental time available for users BL-18B, unlike BL6A2, provides a point focused white beam. This latter feature gives the station time-resolved Laue capability. Special Image Plates (IP) (400mm x 400mm and 400mm x 800mm) and IP scanner are also being developed to allow more effective exposures using Weissenberg and Laue cameras at the station.

PS-01.02.08


We are presently constructing a neutron Laue diffractometer to extend the range of protein structures which can be measured to atomic resolution by neutron diffraction. Finding a two-dimensional detector with digital readout, spatial resolution of 1nm, good dynamic range, and a large angular coverage has become a significant part of the project.

One possible solution is to have an array of position sensitive photomultiplier tubes, each with a Li glass scintillator, around the sample.

We have tested a Hamamatsu 3" square tube with a Nuclear Enterprises 902 scintillator greased onto its front surface. Light produced by the scintillator falls on the photocathode and the resulting electron shower is amplified by a chain of dynodes and subsequently detected on an anode grid at the back of the tube. The data reading system consists of delay lines which are connected to each set of anode wires, along which the electron pulses travel simultaneously. By timing the arrival of the pulses at each end of the delay lines, the X,Y coordinates of the original neutron arrival at the scintillator can be found.

The integrated intensities of reflections have been measured on a four-circle neutron diffractometer with the tube and with a 'normal' BF3 monodetector. Using a 2mm thick scintillator, the tube has been found to be more than 60% efficient at a neutron wavelength of 0.84A, and to have a resolution better than 1nm.

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PS-01.02.09

A NEUTRON-SENSITIVE TV IMAGE INTENSIFIER SYSTEM. By J. G. Smith* and J. B. Davidson, Oak Ridge National Laboratory, Oak Ridge, TN 37830.

A neutron-sensitive TV-image-intensifier system has been in use at the ORNL HFIR reactor for a number of years. This system, though only qualitative and somewhat bulky, has been extremely useful in monochromator alignment, sample alignment in environmental containers, and in the characterization of samples -- single crystal and polycrystalline -- all in real time. With the recent development of miniature CCD cameras coupled with PCs and frame grabbers and imaging processing techniques, the new systems are almost off-the-shelf items and can be readily assembled in-house. While not quite at the quantitative stage for accurate data accumulation, processing, and analysis, the new systems are compact, easy to use, and relatively inexpensive.
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PS 01/02.10 MULTIPLE SMALL-ANGLE SCATTERING— A BLESSING IN DISGUISE? by S. Mazumder* and A. Sequeira, Solid State Physics Division, Bhabha Atomic Research Centre, Bombay-85, India.

In small-angle scattering (SAS) studies, multiple scattering is generally viewed as an unavoidable complication. The common practice as it stands today, is to obtain correction factors to eliminate the effect of multiple scattering in analysing the scattering data. A recent formalism on multiple SAS (1 Mazumder S. and Sequeira A., Pramana, 1992, 38, 95-159) indicates the following facts which we consider to be blessings in disguise if properly exploited:

By merely scaling down the wave-vector transfer, the Guinier law can be extended for multiple SAS. Porod's law remains invariant under multiple scattering as far as the functional dependence of the scattered intensity on wave-vector transfer is concerned. For polydisperse systems, the extractable structural parameters are the moments $<R^2>/<R^2>$ and $<R^2>/<R^2>$ where $R_i$ is linear dimension of the $i$-th type of inhomogeneity. The averaging is over the population density.

In this paper, it is emphasized that the second moment of the single scattering cross-section manifests predominantly in the Guinier regime of the multiple scattering profile. Consequently, so far as the curvature in the Guinier regime is concerned, multiple scattering profile does not bear the signature of the interparticle interference function to any significant level. The insignificance of the interparticle interference function in multiple scattering profile can be exploited to extract particle size distribution of inhomogeneities in dense systems with the help of variational technique like the maximum entropy. It is to be noted here that in a traditional SAS study, the extraction of particle size distribution from dense systems is not possible due to interparticle interference effect.

A methodology for extraction of integral and differential parameters from a multiple scattering profile, as also for the elimination of the effect of multiple scattering when it is a nuisance will be presented. The results of an experimental investigation on two bimodal alumina samples demonstrating the validity of some of the above mentioned aspects will also be discussed.

PS 01/02.11 OMEGA ENERGY FILTERING TEM: APPLICATIONS IN QUANTITATIVE ELECTRON DIFFRACTION. C. Dettinger and J. Mayer, Max-Planck-Institut für Metallforschung Stuttgart, Germany.

With imaging energy filters becoming commercially available in transmission electron microscopy many of the limitations of conventional TEM instruments can be overcome. Energy filtered images or diffraction patterns can now be recorded without scanning using efficient parallel (2-dimensional) detection. We have evaluated a prototype of the Zeiss EM 912 Omega, the first commercially available electron microscope with integrated imaging Omega energy filters. In quantitative electron diffraction the filter is used to remove the inelastically scattered electrons (elastic or zero-loss filtering) and by this quantifiable intensity data without background can be obtained. In selected area diffraction (SAD) weak reflections can be recorded even in thick samples. Another example is the determination of amorphous structure factors of amorphous materials. The most accurately quantifiable data can be obtained by elastically filtered convergent beam electron diffraction (CBED). Structure factor amplitudes and phases can be determined very accurately. For phase measurements in non-centrosymmetric crystals, three beam patterns have to be used. Two dimensional energy filtered data are needed which (without scanning) can only be obtained with an imaging filter and a CCD camera as (linear) detector. From a whole set of such structure factors the charge density distribution in a crystal can be calculated. Furthermore, in the electron spectroscopic diffraction (ESD) mode of operation the angular distribution of inelastically scattered electrons can be imaged. This can be used in the ALCHIMI method to determine atom positions within a unit cell.

PS 01/02.12 DEVELOPMENT OF CCD-BASED AREA DETECTORS FOR MACROMOLECULAR CRYSTALLOGRAPHY USING SYNCHROTRON AND LABORATORY SOURCES, by Walter G. Philipps, Martin Stalgon, Yuli Li, Daniel O'Malley, Jihui Kim, Renowned Basic Medical Sciences Research Center, Brandeis University, Waltham, MA 02254-0010, Edwin M. Westbroek, Isyvan Naday, Steve Bros, Mary L. Westbroek, Miko Kaino, Argonne National Laboratory, Argonne, Ill. 60439, and James W. Illingworth, Cold Spring Harbor Laboratory, Cold Spring Harbor, N.Y. 11724, U.S.A.

We are developing CCD-based area detectors for collecting macromolecular crystallography data using synchrotron and laboratory sources. The basic unit of our detectors is a module which consists of a deaerifying fiber optic taper with a phosphor x-ray converter bonded to the larger face of the taper and a CCD bonded to the smaller face. In order to achieve a large area, detectors are assembled from a number of identical modules. Currently, two detectors are being developed: (1) a high-performance detector for synchrotron applications, and (2) a detector in which a variable number modules can be assembled for a range of applications. The first detector is designed to have a large area, high spatial resolution, high DQE and fast frame rate. These goals are achieved by using a fixed 3x3 array of nine 5 x 5 cm square modules, forming a 15x15 cm area. Each module has a taper demagnification of 2:1, and uses a 1024x1024 pixel Tektronix CCD. As a result this detector has 3972x3972 50um pixels and a high DQE. The second detector is designed so that a single module will form a useful instrument at a reasonable cost, while multiple modules can be used to increase the efficiency of data collection. Each module has a 5x10 cm front surface and a taper demagnification of 4:1, providing a pixel size of 100 μm with a 1024x1024 Tektronix CCD. Because of the larger taper demagnification used in this detector, the cost per unit area is lower, and the performance (as measured by the DQE) is decreased. In both detectors the CCDs are read out in parallel using two amplifiers or each CCD, with a total readout time 1.75 s for the array of up to 9 modules. The pixels can be binned, reducing the readout time to 0.4 s.