POLYCAPILLARY OPTICS BASED NEUTRON FOCUSING FOR SMALL SAMPLE NEUTRON CRYSTALLOGRAPHY

W.M. Gibson[a], H.H. Chen-Mayer[b], D.F.R. Mildner[b], H.J. Prask[b], A.J. Schultz[c], R. Youngman[a], T. Gnäupel-Herold[b], M.E. Miller[c], and R. Vitt[c]

a) X-Ray Optical Systems, Inc., Albany, NY, b) National Institute of Standards and Technology, Gaithersburg, MD, c) Argonne National Laboratory, Argonne, IL

Neutron diffraction is a powerful tool for analysis of crystal structures. Whereas the more widely used x-ray diffraction measures the electron density distribution from which the atomic structure is inferred, neutrons scatter from atomic nuclei and therefore determine the atomic positions directly. Moreover, neutrons can determine positions of very light atoms such as hydrogen, which are nearly invisible to x-rays because of their low electron density. By isotopic tagging, it is also possible to identify active sites and, because of the magnetic moment of the neutron, to determine magnetic ordering.

However, applications of neutron diffraction have been severely limited by the low intensity and limited number of available neutron beams. In recent years, extensive work has been carried out to increase the efficiency of neutron diffraction measurements especially the development of large area position sensitive detectors and the time-of-flight "pseudo-Laue" method which permits a broad wavelength bandwidth to be used. Even with these improvements, structural measurements require large crystals, long measurement times (weeks) or both. In many important cases, as with analysis of macromolecular structures, and measurement of atomic structure at ultra high pressure or low temperature, the sample size is limited to less than 1 mm^3, virtually precluding the use of neutron diffraction as a useful tool

Neutron focusing with polycapillary focusing optics could help overcome this limitation. As a first step to investigate the possibility to use focused neutron beams for small-sample crystallography or high pressure structural studies, we have investigated the neutron focusing properties of a polycapillary focusing optic. We have used neutrons at five selected wavelengths from the BT-8 neutron monochromator at the National Institute of Standards and Technology and a continuous neutron spectrum from ~1->5 Å wavelength from the Single Crystal Diffraction (SCD) facility at the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory. The dependence of the transmission efficiency, focal spot size and gain on the input angular distribution and neutron wavelength were measured. We also have carried out preliminary diffraction measurements with the polycapillary focusing optic on the IPNS-SCD facility at ANL. The results of these studies and prospects for the future will be discussed.