

**PS01.02.09 CURVED IMAGE-PLATES FOR SYNCHROTRON RADIATION HIGH RESOLUTION POWDER DIFFRACTION AND STUDIES OF AMORPHOUS SYSTEMS** G.Bushnell-Wye\*, J.L.Finney+, R.O.Piltz+, J.K.Walters+, J.D.Wicks+, \*CLRC, Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK, +Department of Physics & Astronomy, University College London, Gower Street, London WC1E 6BT, UK

We report the development of two curved image-plate cameras aimed at extending the use of high intensity synchrotron radiation by increasing experiment throughput and by enabling new possibilities in structural studies of crystalline powders and amorphous materials. By replacing incremental scanning of a detector over a wide angular range with a detector system capable of recording the complete diffraction pattern in a single exposure, data collection times have been reduced from hours to minutes. This improves the sample turn round time considerably and will lead to greater access to a scarce resource. Moreover, it no longer requires the sample to be in a steady state: chemical reactions and physical processes could be studied by recording the diffraction pattern as a function of time as the imaging phosphor screen is translated during the experiment. Powder patterns collected in this way would retain high resolution characteristics and allow structure refinement of intermediate phases. Investigation of point to point variations in glassy materials should be possible using a 0.5 mm square beam. Progress in the commissioning of a high resolution camera (larger radius, angular range 70°) for powder diffraction and a low resolution camera (smaller radius, angular range 130°) for studying amorphous materials is described.

**PS01.02.10 FIRST RESULTS FROM THE NEW DARESBUURY CHEMICAL/MATERIALS SINGLE-CRYSTAL DIFFRACTION BEAM-LINE 9.8.** William Clegg Department of Chemistry, University of Newcastle, Newcastle upon Tyne NE1 7RU and Daresbury Laboratory, Daresbury, Warrington WA4 4AD, U.K.

At the time of abstract submission the new high-flux single-crystal diffraction station at Daresbury is almost ready for commissioning. It is designed with a horizontally focussing triangular monochromator and vertically focussing mirror (constrained by the available space close to the tangent point on the original Wiggler of the SRS), and is expected to deliver up to  $10^{13}$  photons/second at the sample. A wavelength range of 0.3-1.5 Å is accessible.

The station is equipped with a range of goniometer and detector systems. An Enraf-Nonius CAD-4 diffractometer provides for serial measurement of individual reflections. A MARresearch image plate is available, and the addition of a Siemens SMART CCD system is currently being considered, following tests carried out at ESRF. Facilities for low-temperature data collection are already in place (Oxford Cryostream), and equipment for high temperature and high pressure are being developed.

Some results from five months of commissioning use will be presented. These will include a wide variety of samples provided by many research groups supporting the funding application for the station, working in diverse fields of chemistry and materials science. Commissioning will include an assessment of the relative merits of the available goniometer/detector systems in a synchrotron environment.

**PS01.02.11 X-RAY CAPILLARY OPTICS, TEST AND APPLICATIONS ON AN UNDULATOR BEAM LINE AT ESRF.** P.Engström, C.Riekel. ESRF, B.P.220, F38043 Grenoble Cedex, France.

With the start of the third generation synchrotron radiation sources for hard X-rays like ESRF, APS and Spring-8 a demand for new types of focusing optics has evolved. One of the possible optics is the X-ray Capillary Optics (XCO) which is based on a very simple principle of total reflection. By letting the X-ray beam enter the hollow capillary and by multiple reflection being transmitted and at the same time letting the diameter of the hole decrease in size an intensity increase being achieved. In this way beams of 1 μm or smaller can be reached. We will present a number of test of XCO on the undulator based micro focus beam line of ESRF under different conditions. We will also show how one can remove a lot of the background for XRD, WAXS and high angle SAXS. We will show a couple of applications in order to illustrate the potential of this optics. We have with this method reached over  $10^{10}$  photons/s/μm<sup>2</sup> with  $2 \cdot 10^{-4} \Delta E/E$  at about 13 keV.

**PS01.02.12 RESONANCE SCATTERING STUDIES OF MIXED VALENCE MANGANESE COMPLEXES** V. Kezerashvili, A. Darovsky, X3 beamline, NSLS, Brookhaven National Laboratory, T. Weyhermüller, Max-Planck-Institut für Strahlenchemie, Mülheim, Germany, P. Coppens, Chemistry Department, SUNY at Buffalo

Manganese mixed-valence complexes model the catalase enzymes and photosystem II, which catalyzes the water oxidation reaction. We have studied three mixed valence complexes in an application of *valence-specific diffraction*, which allows site-specific assignment of oxidation state and mapping of  $f'(E)$  for individual atoms. Peaks on imaging plates were integrated with the program HIPPO<sup>1</sup>. The complexes are (a): Mn(IV)(ttacn)(μ-O)<sub>2</sub>(μ-MeCO<sub>2</sub>)Mn(III)(MeCO<sub>2</sub>)<sub>2</sub>, ttacn=1,4,7-trimethyl-1,4,7-triazacyclononane, (b): [(ttacn)Mn(II)(μ-O)(μ-pivalonato)<sub>2</sub>Mn(III)(ttacn)](ClO<sub>4</sub>)<sub>2</sub>, (c): [(dtne)Mn(IV)(μ-O)<sub>2</sub>(μ-MeCO<sub>2</sub>)Mn(III)(Bph<sub>4</sub>)<sub>2</sub>, dtne= di-1,4,7-triazacyclononane 1,2-ethylene, ph=phenyl. In (a) a definite shift in edge energy is observed, somewhat smaller, but similar to the shift for μ-dioxo-(Mn(2,2'-bipyridyl)<sub>2</sub>)<sub>2</sub>(BF<sub>4</sub>)<sub>3</sub>·3H<sub>2</sub>O (d)<sup>2</sup>. The pre-edge feature in the fluorescence spectrum is reflected in the Mn(IV), but not in the Mn(III) curve, indicating that the transition to a free bound state occurs at the former atom. For (b) and (c) the edge shifts appear much smaller, implying a smaller difference in electron binding energies, and therefore a smaller difference in net charge between the two atoms. Based on the current results the sequence of the magnitudes of the edge shifts in the III-IV complexes is (d)>(a)>(c), while the Mn-O bond asymmetries are in the order (a, 0.098 Å)>(d, 0.069 Å)>(c, 0.048 Å).

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