



Research Activities in Materials and Biostructure at BL12B2

The basic design concept of BL12B2 is to complement the three wiggler beamlines 17A, B & C of TLS and extend their capabilities, especially to use higher energy X-rays. There are four experimental stations in operation now: X-ray absorption spectroscopy, powder X-ray diffraction, high resolution X-ray scattering, and protein X-ray crystallography. A layout of the beamline is shown in Fig. 1.

The demand to use BL12B2 has been very high since its opening. By the end of 2001, 22 experimental runs had been carried out on this beamline, with 59 users outside of SRRC participating in the experiments. In category of research fields, 28% beamtime was allocated to XAS, 28% to X-ray scattering, 14% to powder X-ray diffraction and 15% to protein crystallography. In this report we highlight some results obtained from BL12B2. For more detail information, the readers are referred to the Research Abstracts of the Annual Report.

X-ray Absorption Spectroscopy

On BL12B2, the monochromatic X-rays are

selected by a DCM and focused by a toroidal mirror. The beamline is capable to deliver synchrotron X-rays with energies from 6 to 80 keV. The XAS station is equipped with standard ion chambers, Lytle detector, solid state detector, and a low-temperature sample stage (down to 10 K). With the availability of high-energy X-rays, it is particularly useful on studying the absorption spectrum of heavy elements. For instance, a group led by Prof. B.-J. Hwang of National Taiwan University of Science and Technology investigated the formation and growth mechanism of bimetallic Pd/Ag nano-particles in microemulsion using in-situ EXAFS. They were able to study the particle formation with time. Prof. Hwang's group is also doing in-situ EXAFS studies of electrodes of Li-batteries and fuel cells. (See B.-J. Hwang's article in Research Highlights.)

Powder X-ray Diffraction

A curved image plate (model:IPR-420) is installed on BL12B2 for powder X-ray diffraction measurements. This end station has been used by material chemists in crystal structural studies. For



Fig. 1: Beamline layout of BL12B2.

example, Prof. K.-J. Chao's group of National Tsing Hua University took the advantage of the availability of high energy X-rays to study the formation of bimetallic AuPt nanowire grown inside zeolite cavities. Another example is from Prof. Y. Wang's group of Taiwan University on the study of a high- T_c superconductor related compound ruthenate. Their X-ray measurements allow them to map out the charge density distributions of the compound (see Fig. 2).

X-ray Scattering

BL12B2 is equipped with a 6-circle diffractometer for high resolution scattering studies. Prof. D. Y. Noh's group of KIST, Korea has performed anomalous X-ray scattering on a series of InGaN multiquantum wells. They were able to identify the concentration of In in the crystalline lattice independent of lattice strain (see Fig. 3). Another example is from Dr. C.-H. Du of

SRRC and Prof. S.-L. Chang of National Tsing Hua university, who applied X-ray multiple diffraction to investigate the phases problem in the low dimensional CDW materials. Further experiments are planned to apply an electric field to the sample to probe the dynamic behavior of the charge modulation.

X-ray Protein Crystallography

Through a joint effort between JASRI and SRRC, a protein crystallography station at BL12B2 was installed in August 2001. This station is equipped with an ADSC Quantum 4R CCD detector and a high-speed data network system for data acquisition and reduction. The phasing studies of macromolecular crystals by Single/Multiple Anomalous Dispersion (SAD/MAD) method have already been carried out on this station. For example, Dr. C.-J. Chen's group of SRRC applied SAD at the K-edge of Fe on bacteria *Desulfovibrio gigas*, and successfully solved the crystal structure with ultra-high resolution of 0.68 Å (see Fig. 4).

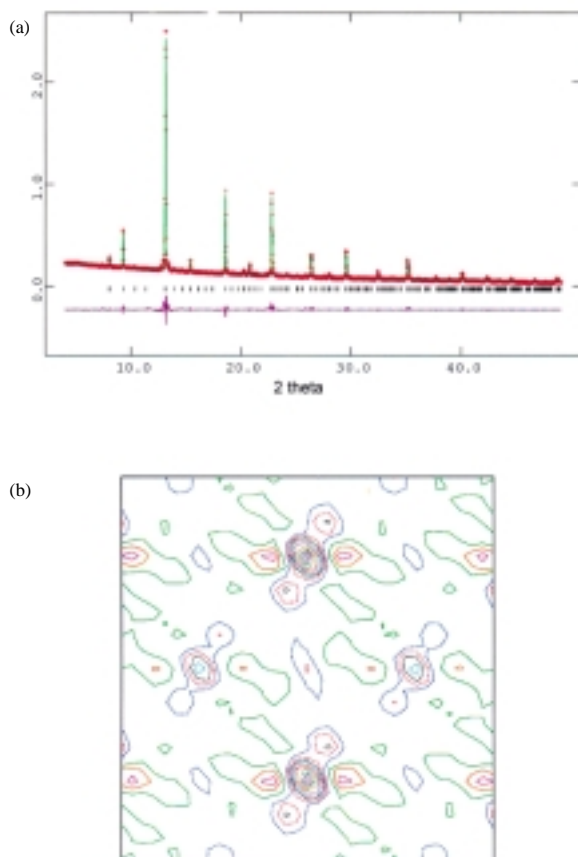


Fig. 2: X-ray powder diffraction results obtained from $Ba_2HoRu_{0.9}Cu_{0.1}O_6$ with a curved image plate: (a) X-ray powder pattern; (b) charge density.

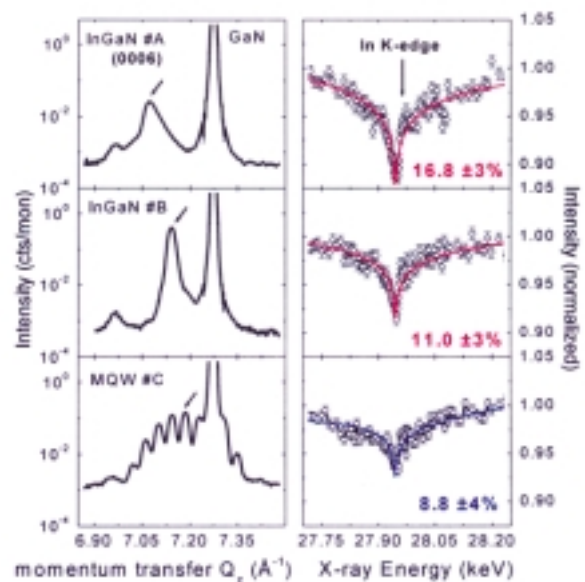


Fig. 3: Anomalous X-ray scattering profiles measured at Bragg peak (0 0 6) across In K-edge for two single-quantum well samples (samples # A and B) and a multiquantum-well sample. The depth of the intensity cusp is very sensitivity to the indium composition.

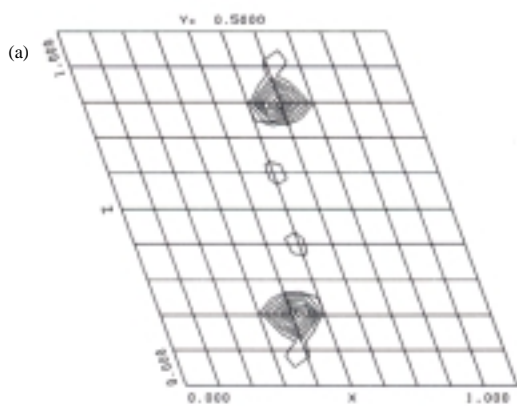


Fig. 4: The structure of an iron-sulfur protein Rubredoxin solved by Fe-SAD/MAD method and refined to 0.7 Å resolution: (a) Fe anomalous difference Patterson map; (b) The structure of the protein where Fe (III) ion is shown as the red ball.

Acknowledgements

We thank SRRC X-ray group for the installations of three end stations: J. F. Lee for XAS, H. S. Sheu for powder X-ray diffraction, and C. H. Hsu for 6-circle diffractometer. We thank H. Moriyama of JASRI and Y. C. Jean, Y. S. Huang, and C. H. Chao for the installation of the protein crystallography station.

Authors:

M. T. Tang, C. H. Du, and K. S. Liang
Synchrotron Radiation Research Center, Hsinchu, Taiwan

Publications:

- M. T. Tang, T.-E. Dann, C.-C. Chen, K.-L. Tsang, C. T. Chen, and K. S. Liang, Nucl. Instrum. Meth., **A467-468**, 719 (2001).
- C. M. Yang, H.-S. Sheu, and K.-J. Chao, Adv. Func. Mater., **12**, 143 (2002).
- J. F. Lee, M.-T. Tang, W.-C. Shih, and R. S. Liu, Materials Res. Bull., **37**, 555 (2002).