BL12B2
APCST BM

In year 2002, the Taiwan Beamline BL12B2 has reached up to its full speed operation. This can be realized in two respects; the rapid increase in the number of user-run on one hand and the fruitful output from the beamline on the other hand. Compared to year 2001, the number of user-run at BL12B2 increased about double in year 2002, that is 190 user-runs in year 2002, compared to 95 user-runs in year 2001. Owing to the completion of the joint protein crystallography station in the early February of 2002, the protein users not only attribute more research activities at BL12B2, but also allocate about 40% of the total user beamtime, resulting a redistribution in beamtime allocation. The beamtime allocation to various user's applications is shown in *Figure 1.* As for the beamtime allocated to each experiment, in average, the protein proposals were granted for 1-2 days, and the EXAFS 3 days, the powder X-ray diffraction 4days and the X-ray scattering 5days. There was 18% of total user beamtime allocated to JASRI, specifically for the Microgravitorial and Industrial Proteomics with Synchrotron radiation (MIPS) project, to fulfil the contract condition between APCST and JASRI. We will outline some of the works done at BL12B2 in 2002 and the reader are encouraged to refer to the experimental results published in SPring-8 User Report No. 9 (2002A) and No. 10 (2002B).

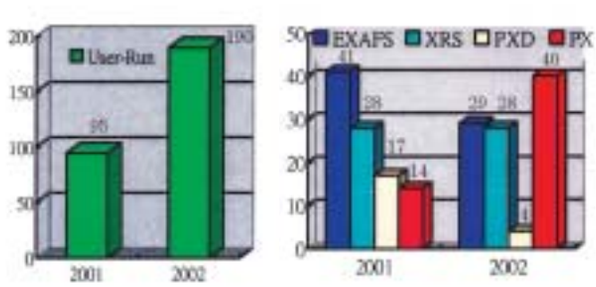

Figure 1 A comparison of user statistics at BL12B2 in year 2001 and 2002. The user-run has increased rapidly since the beamline opened to public in September 2001. A redistribution among various user's fields is found after the completion of protein station in February 2002.

1. Materials Research

The BL12B2 has ever since the completion provided a manifold detecting environment for variously prepared sample systems in diverse disciplines. Although not arranged in advanced, in year 2002 several materials researches were strongly related to nano-technology and science. These researches have utilized the X-ray Absorption Spectroscopy for short range structural detection and the X-ray scattering/diffraction for long range order measurements as well. More over, the users combined these two techniques to detect and quantitatively determine the contribution from specific element within nano size regime, and sometimes under non-ambient environment such as high pressure. Besides, a unique technique, the X-ray multiple diffraction, for recording the phase shift resulting from an externally applied electric field to a quasi one-dimensional crystal will also be described briefly.

1-1 EXAFS

The EXAFS station has been a busy station since the early commissioning period of beamline. This year, several long term projects have been continuing at the station, including groups of Prof. K-J Chao (NTHU), Prof. T-P Perng (NTHU), Prof. B-J Hwang (NTUST) and Prof. C-Y Mou (NTU). A new setup by adopting EXAFS technique, led by Prof. C-M Lin (NHTC), has been preliminarily conducted at BL12B2 in study the high pressure phase transition of MnTe, from which, combined with Raman scattering spectrum and powder X-ray diffraction, the long suspected structural phase transition of MnTe at around 6.0 GPa was experimentally confirmed.

1-2 Anomalous X-ray scattering study on self-assembly quantum dots

The self-assembled quantum dots (QD) have recently attracted intensive research interests due to their potential impact to future nano electronic industry. Yet to fully understand the physical characters of QDs, a precise structural probing tool is rather missing. Years ago, the surface X-rays scattering has been applied to

provide an atomic resolution probe to mapping the strain distribution inside the dots, while, the distribution of the contented composition is rather poorly determined. By applying the anomalous X-ray scattering at the Ga K-edge to the weak reflection (200) of the QDs, Dr. C-H Hsu (NSRRC) 's group has recently developed an element sensitive technique to precisely map the In/Ga composition distribution in the self-assembly $In_{0.5}Ga_{0.5}As$ QDs to an estimated factor of 20 times enhancement in sensitivity.

1-3 Observation of the field induced phase deping in the charge density waves of $K_{0.3}MoO_3$.

The phonon - electron interaction in a strongly anisotropic crystal frequently, when lowering beneath transition temperature, results in crystal structural modulation, the so-called charge density wave (CDW) and exhibits abnormal transport behaviours. Analogy to BCS superconductors, the CDW can be characterized by a complex order parameter, that its amplitude explains the transition temperature, while its phase is related to the transport manners. In this study, Prof. C-H Du (Tamkang U.), Dr. M-T Tang (NSRRC) and Prof. S-L Chang (NTHU) and coworkers applied the X-ray multiple diffraction to record the phase shift resulting from the externally applied electric field to the quasi-one-dimensional $K_{0.3}MoO_3$ crystal and unambiguously found the phenomena of deping CDW phases by 40^{o} nearby the threshold applied field.

2. Biostructural Research

The protein crystallography station, a collaborative project between APCST and JASRI, has been thereafter put in action since its completion in February 2002. The end station is equipped with a ADSC Quantum 4R CCD detector and a shared high speed data network system. The schematic drawing of the computer architecture at BL12B2 can be found in SPring-8 年報. Here we outline some fruitful results from the station in 2002.

2-1 Crystal structure of the hyperthermoplilic archael DNA-binding protein Sso10b2 at 1.85 Å resolution by Andrew H.-J. Wang (Academia Sinica)

The families of small, abundant, and basic DNA binding proteins in thermoacidphilic archaea of the genus *Sulfolobus* were first characterized in the 1980s. These proteins can be grouped into three classess according to their molecular sizes (7, 8 and 10 kDa, respectively). Two members of the 7 kDa proteins have been under extensive studies, but little is known about 8 kDa and 10 kDa proteins. *Sulfolobus solfataricus* Sso10b is one of the 10 kDa members. The crystal structure at 2.8 Å resolution of the Sso10b1 has been solved recently. To further explore the function and diversity of the Sso10b1 and Sso10b2 proteins, Prof. A H-J Wang's group present the crystal structure of Sso10b2 from *Sulfolobus solfataricus* at a substantially higher resolution of 1.85 Å than that of Sso10b1, *(Figure 2)*. The Zn-MAD data sets and the high resolution data were collected at BL12B2 and BL17B2 (NSRRC), respectively.

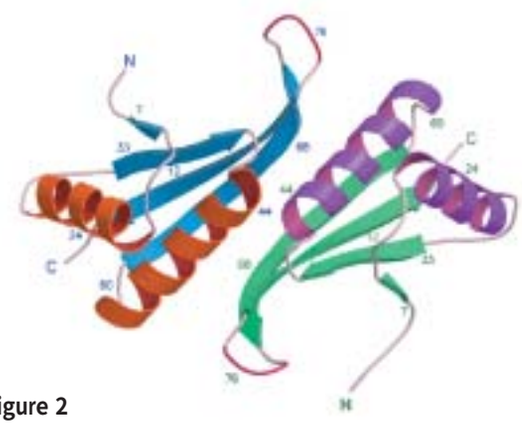

Figure 2

2-2 Structural determination of the yeast cytosine deaminase by Shwu-Huey Liaw(NYMU)

Yeast cytosine deaminase (CD) is an attractive candidate for anticancer gene therapy because of its catalysis of the deamination of the prodrug 5-fluorocytosine into 5-fluorouracil. Recently at BL12B2, Prof S-H Liaw (NYMU)'s group has solved the crystal structure of the enzyme in complex with the inhibitor 2-hydroxypyrimidine at 1.6 Å resolution by the Se-MAD methods. The current model contains residues 8-158 with clear electron density. The protein structure is composed of a central five-stranded β sheet, sandwiched by five α-helices *(Figure3)*.

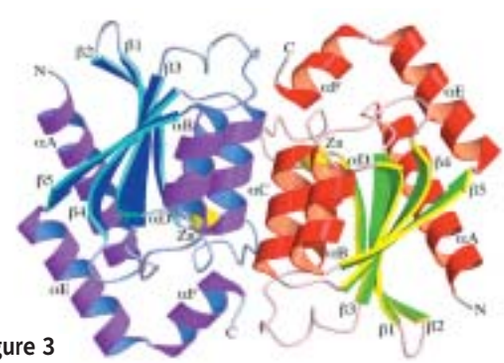

Figure 3

2-3 Crystal structure determination of bio-technique-value proteins and membrane proteins in lipidic cubic phases using synchrotron radiation by Chun-Jung Chen (NSRRC)

Rubredoxin (Rd), a small redox protein, is often purified from anaerobic bacteria where it is thought to be involved in electron transfer processes. Rds from *Desulforibrio desulfuricans* ATCC 27774, which is a kind of anaerobic bacteria are composed of approximately 52 amino acid residues and have a molecular weight of about 6000 Da. They have been isolated and been crystallized at aerobic condition. The structure has been ab initio determined at BL12B2 *(Figure 4)* from X-ray diffraction data by SAD using Fe as the anomalous scatterer. The Rubredoxin crystals diffracted better than 0.68 Å. The data shows they belong to the space group $P2_1$ with cell parameters: a=19.44 Å, b=41.24 Å β=108.46 °.

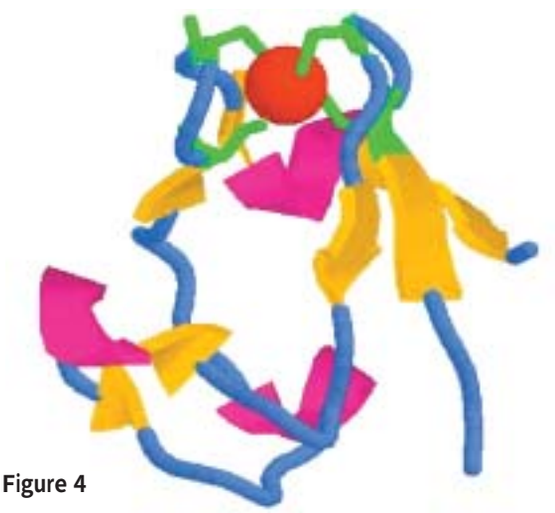

Figure 4

Acknowledgements

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