BL12B2
NSRRC BM

BL12B2 is one of the two contact beamlines based on the collaborative Memorandum of Understanding between National Synchrotron Radiation Research Center (NSRRC, Taiwan), Japan Synchrotron Radiation Research Institute (JASRI), and RIKEN SPring-8 Center (RSC). The user support and end station maintenance of the beamlines have been provided by NSRRC. BL12B2 has been maintained to serve for material science and protein crystallography users since 2000. The schematic layout of the beamline is presented in Figure 1. The beamline is equipped with collimating mirror (CM), double crystal monochromator (DCM), and focusing mirror (FM). The measured spot size and total flux of the beam is about 250 μm square and about $1.5x10^{11}$ respectively at protein end station at 12 keV. Four end stations, EXAFS, X-ray diffraction, X-ray scattering, and protein crystallography (PX) end stations, are equipped inside the experimental hutch of BL12B2.

The EXAFS experiment is measured using two ion chambers at EXAFS table located at most upper stream of the BL12B2 experiment hutch. The users can carry out experiment by placing their sample in between these two ion chambers. Powder x-ray diffraction is measured using image plate at XRD table located next to the EXAFS table. X-ray scattering experiment can be carried out using six circle diffractometer. The sample environment of these two experiments can be changed from 20-400 K. High pressure x-ray diffraction can be carried out using CCD camera at protein crystallography table. Protein crystallography (PX) end station which is equipped with CCD and SPring-8 standard auto sample changer system has been installed since 2009. The user interface software of PX is SPring-8 standard BSS. Remote access capability of this PX system has been tested and operated from 2011. The CCD detector has been upgraded from Quantum 210r to Raynox

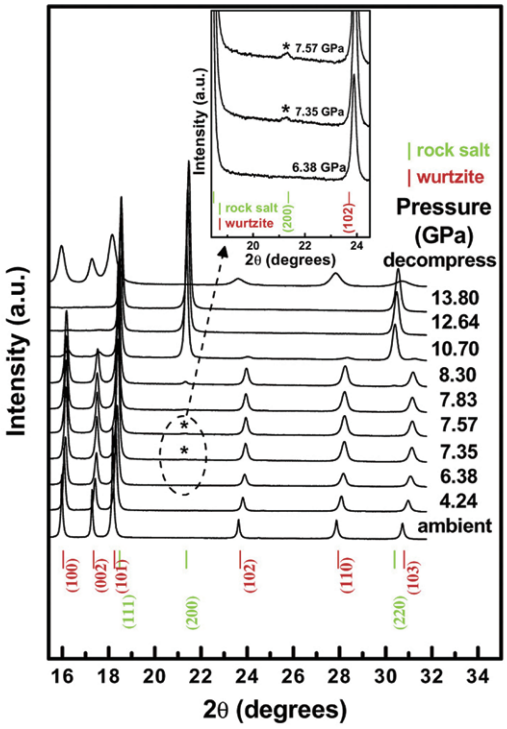

Fig.2 High pressure Angle Dependent XRD of bulk $Zn_{0.98}Mn_{0.02}O$ at elevated and decompresses pressures. Bulk $Zn_{0.98}Mn_{0.02}O$ exhibited a phase transition with an onset pressure of 7.35 GPa marked within the inset. [2]

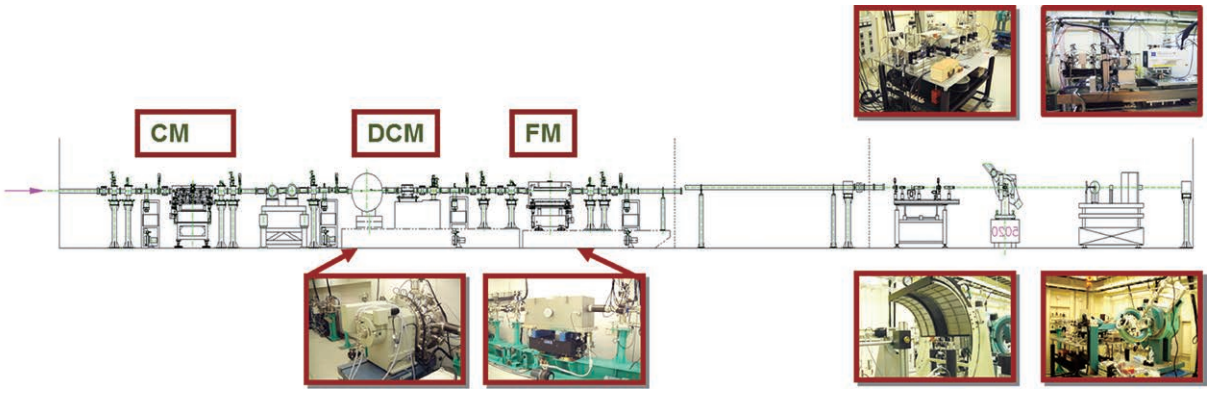

Fig.1 Schematic layout of BL12B2

MX225-HE in 2014. The fast read out and wide detection area of the new detector will help user to collect high quality data.

EXAFS, x-ray diffraction, x-ray scattering end stations are serving for material science users. The experiments are covering wide area of material science topics, such as environmental science, nano science, geophysical science, etc.

In 2014 BL12B2 users have published fifteen papers in SCI (Science Citation Index) journals. The material science and protein crystallography users have published four and eleven papers respectively. Figure 2 shows the selected result from material science user which has observed the phase transition of zinc oxide based ternary compound $Zn_{0.98}Mn_{0.02}O$. Due to its optical and magnetic properties, zinc oxide (ZnO) based ternary compound has attracted extensive research interest over the decades. The results give new insight in the research of this field. Figures 3 and 4 show the selected results from users of protein crystallography. The new direct phase-selection method greatly enhances the success of the subsequent electron-density modification, model building and structure determination

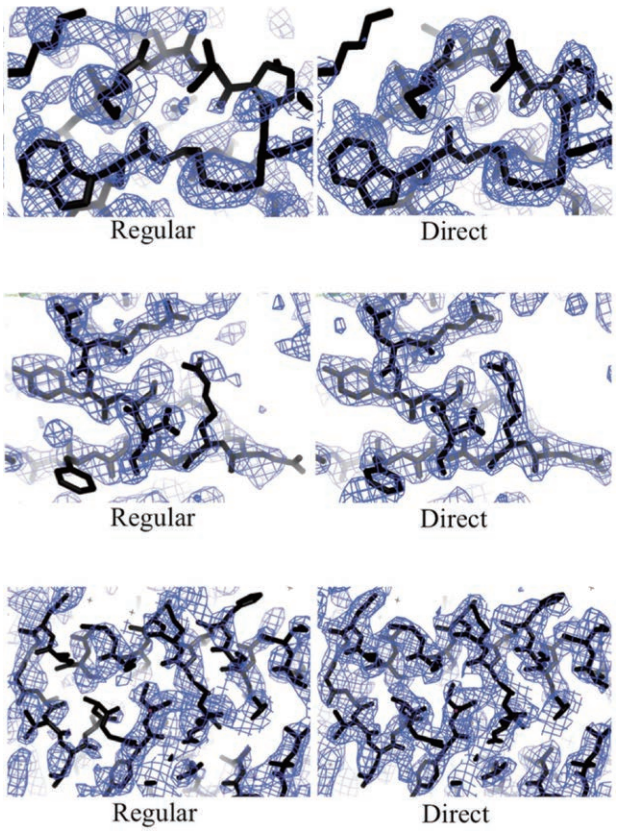

Fig.3 Electron-density maps of lysozyme with S-SAD, insulin with S-SAD and one unknown structure HptB with Se-SAD from the regular method and the direct phase-selection method are shown with the same contour level 1.0 σ in blue. The structures are shown as black sticks. The quality of density maps is significantly improved by the direct phase-selection method. [11]

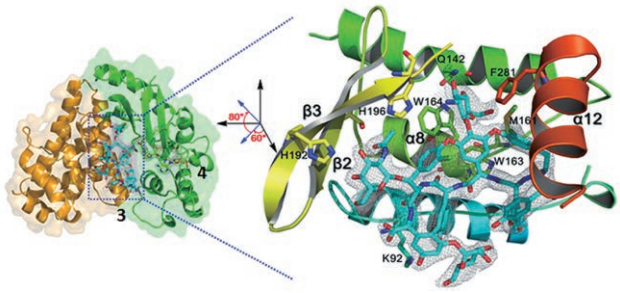

Fig.4 The ternary structure of Orf11* in complex with Tei pseudoaglycone and decanoyl-CoA provide valuable information for developing novel antibiotics to kill vancomycin-resistant enterococcus. The $2F_o$-F_c electron-density maps are contoured at 1.0 σ in grey.[13]

of biological macromolecules, which should benefit the community of structural biology (Fig. 3). The complex structures of Orf11* with Tei pseudoaglycone and decanoyl-CoA provide structural insights for the development of novel antibiotics to kill vancomycin-resistant enterococcus (Fig. 4).

The beam time was shared between material science and protein crystallography users with equal amount. The major users of the B2 beamline in 2013 were from Taiwan. There are also international users from Japan and other place of the world. Users support has been provided by three local beamline scientists and one engineer.

Publications

Material Science

[1] P.-C. Huang, H.-S. Chen, Y.-T. Liu, I.-L. Chen, S.-Y. Huang, H. M. Nguyen, K.-W. Wang, C.-C. Hu, and T.-Y. Chen: "*Oxidation Triggered Atomic Restructures Enhancing the Electrooxidation Activities of Carbon Supported Platinum-ruthenium Catalysts*" CrystEngComm **16** , (2014) 10066.

[2] C.-M. Lin, K.-L. Lin, Y.-K. Chern, C.-H. Hsu, H.-S. Sheu, Y.-F. Liao, Y.-W. Suen, S.-R. Jian, and J.-Y. Juang: "*Pressure-induced Structural Phase Transition in Bulk $Zn_{0.98}Mn_{0.02}O$ by Angular Dispersive X-ray Diffraction*" J. Alloy. Compd. **604** , (2014) 298.

[3] Jang-Jung Wang, Yu-Ting Liu, I-Li Chen, Yaw-Wen Yang, Tsung-Kuang Yeh, Chih Hao Lee, Chi-Chang Hu, Ten-Chin Wen, Tsan-Yao Chen and Tsang-Lang Lin: "*Near-Monolayer Platinum Shell on Core–Shell Nanocatalysts for High-Performance Direct Methanol Fuel Cell*" J. Phys. Chem. C **118**, (2014) 2253-2262.

[4] Ching-Ju Monica Chin, Tsan-Yao Chen, Menshan Lee, Chiung-Fen Chang, Yu-Ting Liu, Yu-Tsun Kuo "*Effective anodic oxidation of naproxen by platinum*

nanoparticles Coated FTO glass" J. Hazard. Mater. **277**, (2014) 110-119.

Protein X-ray Crystallography

[5] C.-K. Chang, M.-H. Hou, C.-F. Chang, C.-D. Hsiao, and T.-H. Huang: "*The SARS Coronavirus Nucleocapsid Protein-forms and Functions*" Antiviral Res. **103**, (2014) 39.

[6] C.-H. Ho, H.-C. Wang, T.-P. Ko, Y.-C. Chang, and A. H.- J. Wang: "*The T4 Phage DNA Mimic Protein Arn Inhibits the DNA Binding Activity of the Bacterial Histone-like Protein H-NS*" J. Biol. Chem. **289** , (2014) 27046.

[7] Y.-C. Hsieh, H.-H. Chiu, Y.-C. Huang, H.-K. Fun, C.-Y. Lu, Y.-K. Li, and C.-J. Chen: "*Purification, Crystallization and Preliminary X-ray Crystallographic Analysis of Glycosyltransferase-1 from Bacillus Cereus*" Acta Crystallogr. F **70**, (2014) 1228.

[8] W. Praditwongwan, P. Chuankhayan, S. Saoin, T. Wisitponchai, V. S. Lee, S. Nangola, S. S. Hong, P. Minard, P. Boulanger, C.-J. Chen, and C. Tayapiwatana: "*Crystal Structure of an Antiviral Ankyrin Targeting the HIV-1 Capsid and Molecular Modeling of the Ankyrin-capsid Complex*" J. Comput.-Aided Mol. Des. **28**, (2014) 869.

[9] C.-H. Chu, L.-Y. Wang, K.-C. Hsu, C.-C. Chen, H.-H. Cheng, S.-M. Wang, C.-M. Wu, T.-J. Chen, L.-T. Li, R. Liu, C.-L. Hung, J.-M. Yang, H.-J. Kung, and W.-C. Wang: "*KDM4B as a Target for Prostate Cancer: Structural Analysis and Selective Inhibition by a Novel Inhibitor*" J. Med. Chem. **57**, (2014) 5975.

[10] Y.-M. Chang, C.-H. Ho, C. K.-M. Chen, M. Maestre-Reyna, M. W. Chang-Chien, and A. H.-J. Wang: "TcaR-ssDNA Complex Crystal Structure Reveals New DNA Binding Mechanism of the MarR Family Proteins" Nucleic Acids Res. 42, (2014) 5314.

[11] C.-D. Chen, Y.-C. Huang, H.-L. Chiang, Y.-C. Hsieh, H.-H. Guan, P. Chuankhayana, and C.-J. Chen: "*Direct Phase Selection of Initial Phases from Single-wavelength Anomalous Dispersion (SAD) for the Improvement of Electron Density and ab Initio Structure Determination*" Acta Crystallogr. D **70**, (2014) 2331.

[12] Y.-C. Luo, C.-H. Wang, Y.-M. Wu, W. Liu, M.-W. Lu, and C.-S. Lin: "*Crystallization and X-ray Diffraction of Virus-like Particles from a Piscine Betanodavirus*" Acta Crystallogr. F **70**, (2014) 1080.

[13] S.-Y. Lyu, Y.-C. Liu, C.-Y. Chang, C.-J. Huang, Y.-H. Chiu, C.- M. Huang, N.-S. Hsu, K.-H. Lin, C.-J. Wu, M.-D. Tsai, and T.-L. Li: "*Multiple Complexes of Long Aliphatic N-acyltransferases Lead to Synthesis of 2,6-diacylated/2-acyl-substituted Glycopeptide Antibiotics Effectively Killing Vancomycin-resistant Enterococcus*" J. Am. Chem. Soc. **136**, (2014) 10989.

[14] X.-W. Zou, Y.-C. Liu, N.-S. Hsu, C.-J. Huang, S.-Y. Lyu, H.-C. Chan, C.-Y. Chang, H.-W. Yeh, K.-H. Lin, C.-J. Wu, M.-D. Tsai, and T.-L. Li: "*Structure and Mechanism of a Nonhaem-iron SAM-dependent C-methyltransferase and Its Engineering to a Hydratase and and O-methyltransferase*", Acta Crystallogr. D **70**, (2014) 1549.

[15] K.-C. Wang, S.-Y. Lyu, Y.-C. Liu, C.-Y. Chang, C.-J. Wu, and T.-L. Li: "*N-acetylhexosamine 1-phosphate Kinases through Multiple Reaction Complexes*" Acta Crystallogr. D **70**, (2014) 1401.

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