MS07.P09

Acta Cryst. (2011) A**67,** C258

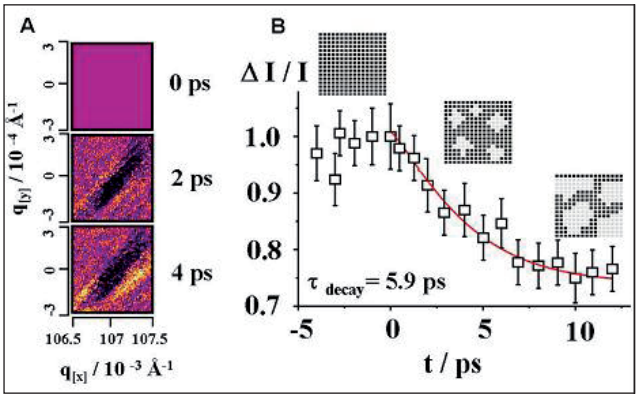
Ultra-fast dynamics of Silver behenate investigated by FEL femtosecond radiation (FLASH)

Wilson Quevedo,[a] Ivan Rajkovic,[a] S*tephan Duesterer,[b] Simone Techert,[a] [a]Max-Planck Institute for Biophysical Chemistry, Department of Structural Dynamics, Goettingen, (Germany). [b]DESY, Hamburg, (Germany).* E-mail: wqueved@gwdg.de

It has been proposed that free electron laser radiation can be used for ultrafast time-resolved x-ray diffraction experiments based on the NIR pulse / FEL probe scheme. We developed a multipurpose vacuum chamber which function is to be used in the pump / probe diffraction experiments with free electron laser (FEL) radiation.

By exciting with optical laser pulses in the near infrared regime (800 nm) it is possible to investigate in silver behenate (AgBh) an optical excitation dependent intensity modulation of its Bragg reflection. The time-resolution of the experiment was about 150 fs. It is assumed that in AgBh the optical laser pulses introduce a structural strain and disorder phase which can be monitored by the intensity modulation of the AgBh Bragg reflection. The strain / disorder results from an ultrafast temperature jump in the system through the non-resonant excitation at 800 nm.

Our studies on model systems like silver behenate has answered the questions of whether it is possible to use soft x-ray free electron laser radiation for studying chemical systems of periodic order and whether it is possible to utilize the time structure of soft x-ray free electron laser radiation for studying the structural dynamics of chemical systems of periodic order, opening a window for the structural studies on nano-periodic systems [1], [2].



Time dependent changes of the Bragg diffraction peak intensities (photo-excited AgBh nanotubes)
A) Intensity difference maps for various time points
B) Time evolution of the integral intensity changes of the Bragg reflection. The creation of the photo-disordered phase and its modelbased on its kinetic analysis are shown in the inset

[1] I. Rajkovic, W. Quevedo, S. Techert, et. al, *Physical Review Letters* **2010**, *104*, 125503. [2] H. Chapman, A.P. Holl, et. al, *Nature,* **2011,** *470*, 73-77.

Keywords: free electron laser, silver behenate, and structural dynamics

MS07.P10

Acta Cryst. (2011) A**67,** C258

iMATERIA, the versatile neutron diffractometer at J-PARC -the current status of iMATERIA -

T. Ishigaki,[a] A. Hoshikawa,[a] M. Yonemura,[b] K. Iwase,[a] D. S. Adipranoto,[a] T. Kamiyama,[b] R. Tomiyasu-Oishi,[b] Y. Morii,[c] M. Hayashi,[c] [a]*Frontier Research Center for Applied Nuclear Sciences, Ibaraki University;* [b]*Neutron Science Laboratory, KEK;* [c]*Ibaraki Prefecture (Japan).* E-mail: toru.ishigaki@j-parc.jp.

Ibaraki prefecture, the local government of the area where J-PARC sites in Japan, has decided to build a versatile neutron diffractometer (IBARAKI Materials Design Diffractometer, iMATERIA [1]) to promote industrial applications for neutron beam in J-PARC. iMATERIA is planned to be a high throughput diffractometer so that materials engineers and scientists can use this diffractometer like the chemical analytical instruments in their materials development process. It covers the d in range $0.18 < d\ (Å) < 5$ with $\Delta d/d = 0.16$ % at high resolution bank, and $5 < d\ (Å) < 800$ with the resolution changing gradually at three detector banks of 90 degree, low angle and small angle. So, this diffractometer covers very wide d-range ($0.18 < d\ (Å) < 800$). It takes several minutes to obtain a 'Rietveld-quality' data for the X-ray laboratory sized sample measured at 1MW. Currently, the beam power is limited for tuning the accelerator (~200kW), so that the measuring time is about 15 to 30 min for standard oxide samples. To promote industrial applications, a utilization system of this diffractometer is required. Since several tens to thousands experiments will be carried out in one year, we have prepared an automatically sample exchange system and large numbers of sample holders. The analysis software is also very important for powder diffraction data, so that we prepare a software package consisting of combination of several powder-diffraction software, include Rietveld analysis software (Z-Rietveld [2]), structural databases and visualization. The construction of iMATERIA was completed and user program was already started since June 2009 for high resolution bank. Because of big earthquake (the 2011 off the pacific coast of tohoku earthquake) in Japan, iMATERIA was also damaged. Currently, restoration workes is progressing. The current status and the recent data of iMATERIA include low angle bank and small angle bank will be reported.

[1] T. Ishigaki et. al., *Nucl. Instr. Meth. Phys. Res. A,* **2009,** *600,* 189-191. [2] R. Oishi, et. al., *Nucl. Instr. Meth. Phys. Res. A,* **2009,** *600,* 94–96.

Keywords: neutron, diffractometer, powder diffraction

MS07.P11

Acta Cryst. (2011) A**67,** C258-C259

Towards macromolecular crystallography beamlines at NSLS-II

D.K. Schneider,[a] R.M. Sweet,[a] M. Sullivan,[b] D. Stoner-Ma,[a] V. Stojanoff,[a] A. Soares,[a] W. Shi,[b] H. Robinson,[a] A. Orville,[a] Q. Liu,[c] J. Lidestri,[c] J. Jakoncic,[a] A. Héroux,[a] W.A. Hendrickson,[c] M. Chance,[b] M. Allaire,[a] and L.E. Berman,[a] [a]*Brookhaven National Laboratory, Upton, NY 11973, (USA).* [b]*Case Western Reserve University, Cleveland, OH 44106, (USA).* [c]*Columbia University and New York Structural Biology Center, New York, NY 10032, (USA).* E-mail: schneider@bnl.gov

Anticipating the unprecedented brightness and flux at the National Synchrotron Light Source-II, we are exploring methods and techniques that will benefit crystallographers to optimally use an initial complement of specialized instruments for macro-molecular crystallography.

At the micro-focusing beamline, FMX, with a beam size of 1–20 µm, one experimental challenge will be the routine delivery of small crystals into the focal spot. Intended to receive the most challenging samples, the beamline may also support acoustic ejection of droplets with passenger crystals onto meshes, followed in the beam by grid search, which has been shown by several of us to be a highly effective micro-crystal handling method.