SLS Symposium on

Nanomagnets and time resolved measurements

Tuesday, October 9, 2018

10:00 to 11:45, WBGB 019

10:00 Artificial Spin Ice Inspired Computation using Nanomagnets
Hanu Arava, P. M. Derlet, J. Vijayakumar, J. Cui, A. Kleibert and L. J. Heyderman

10:30 Recent developments in computational methods for two-dimensional serial femtosecond crystallography: paving the way to the time-resolved study of large-scale movements in membrane proteins
Cecilia Casadei, K. Nass, A. Barty, C. Padeste, D. Ozerov, L. Sala, M. Coleman, X-D Li, M. Frank and B. Pedrini

11:00 Coffee break

11:15 Time resolved X-ray spectroscopy of Nitrosyl-myoglobin in physiological solution
Dominik Kinschel, C. Bacellar, O. Cannelli, B. Sorokin, F. A. Lima, G. Mancini, W. Gawelda, P. Zalden, S. Schulz, J. Budarz, D. Khakhulin, Y. Obara, J. Nishitani, H. Ito, T. Ito, N. Kurahashi, C. Higashimura, S. Kudo, C. Bressler, C. Milne, T. Suzuki, K. Misawa and M. Chergui

Artificial Spin Ice Inspired Computation using Nanomagnets

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Computation using nanomagnets has the advantage of being a low power solution to current CMOS based technologies and is interesting for "beyond CMOS" applications. Here, we present an alternative design to perform Boolean logic using nanoscale magnets. Within this new design, we introduce nanomagnets in a loop scheme as building blocks, which can be considered as a zero dimensional implementation of the artificial square ice. For any computational technology to be complete, it would need two basic elements: (i) a channel to transport information and (ii) a logic gate to perform computation. Here, a 1D representation of the square ice, a square loop chain, was implemented to serve as a "channel" to transport information and logic gates based on the loop structures were designed based on the energy levels associated with different magnetic vertex charges in an artificial square ice. Each logic operation corresponds to a truth table (such as NAND), and is a consequence of the minimization of dipolar energy associated with the magnetic moment rearrangements. We employed synchrotron X-ray PEEM (Photo-Emission Electron Microscopy) to verify the logic operations that were driven by a thermal protocol. We were successful in obtaining an output from a defined input across a maximum tested chain length comprising of 19 square rings. In addition, we tested over 2000 logic gates and experimentally observed that ~94% displayed correct gate operation.

Time resolved X-ray spectroscopy of Nitrosyl-myoglobin in physiological solution

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Myoglobin is a small protein consisting of a single polypeptide chain of 153 amino acid residues and a heme group as its active center, which consists of a porphyrin ring with an Fe atom in its center. It plays a central role in many biological functions based on detection, transport, release and/or binding of molecular ligands such as O_2, CO, NO, CN, etc. The unligated high-spin form (deoxyMb) binds the ligand at the Fe center of the porphyrin, leading to a change to the planar low-spin ligated form, which is the origin of the respiratory Tense to Relaxed state of the protein. Since, the latter is invariant, it seems ligation causes differences in spin, electronic configuration and geometric structure that determine the role of each ligand.

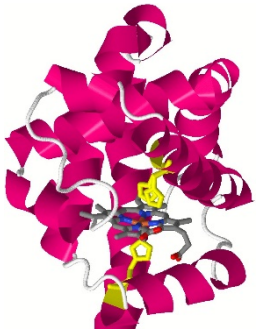

Figure 1: Structure of Myoglobin

Nitrosyl-Myoglobin (MbNO), in particular, is not entirely understood despite its biological relevance as it controls various neurophysiological responses. The ultrafast photodissociation of low spin, planar MbNO leads to the high-spin deoxyMb. However, part of the population undergoes recombination on multiple timescales (from sub-ps to 100s ps) and formation of a high-spin domed ligated MbNO is accepted as one of the intermediates on the way back to the planar form. Previous X-ray absorption studies with 70 ps resolution supported the latter hypothesis, but the nature of the earlier time kinetics is unclear. In particular, is the relaxation back to planar a cascade via spin states or is it due to steric hindrances? In order to elucidate these aspects, we combined femtosecond Fe K-edge X-ray absorption spectroscopy (XAS) with X-ray emission spectroscopy (XES) and X-ray diffuse scattering (XDS) at the FXE beamline of the European-XFEL (Hamburg) and at SACLA (Japan). XAS probes the unoccupied density of states (DOS) and the local structure around the Fe atom, while XES the occupied DOS and the spin state of the intermediates. XDS allows to unravel structural changes of the protein structure. This is the first time these three methods are combined together to investigate biological systems and we will present our results from these measurements and cast them in the context of on-going studies of biosystems at XFELs.

Recent developments in computational methods for two-dimensional serial femtosecond crystallography: paving the way to the time-resolved study of large-scale movements in membrane proteins

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Serial femtosecond crystallography (SFX) is gaining increasing visibility in the the structural biology community because of the unprecedented opportunity of observing molecules in action. Ambient-temperature pump-probe studies of biological molecules are now possible using ultrashort and ultrabright X-ray pulses from free electron lasers, which allow serial data collection in a diffract-before-destroy mode. This method has proved capability of detecting small-scale molecular movements - ranging from side chain movements to cofactor isomerizations - happening on a broad range of time scales. Nevertheless large-scale motions may be sterically hindered in three dimensional (3D) crystals [1] and may not be revealed in a time resolved SFX experiment.

We present here the opportunities offered by two dimensional (2D) crystals *i.e.* 2D periodic arrays of molecules, whose diffraction is measured in a serial fashion. The loose packing in 2D allows wide molecular movements (in the range of a few Å). The challenges in treating the diffraction data are essentially two-fold: (i) monolayers are intrisecally weak scatterers and (ii) intensities from thousands of individual crystals need to be merged and modeled along Bragg lines in reciprocal space. Regarding point (i), we showed in a recent publication [2] how the intrinsic limitation in the signal to noise ratio of the diffracted intensities can be efficiently dealt with by exploiting the high redundancy of the experiment, specifically by summing equivalent portions of images across the data set, leading to the extension of the resolution limit of the usable data. As for point (ii), we successfully reconstructed 3D diffraction intensities along Bragg lines in reciprocal space and we showed that they are meaningful. The presentation will focus on our latest computational developments for data treatment, in particular with respect to the challenges summarised in point (i) and (ii). We developed dedicated processing code in Python, where concepts from traditional X-ray crystallography (lattice identification, lattice parameter refinement), 3D-SFX (merging of images from individual crystals affected by indexing ambiguity, intensity scaling) and 2D electron diffraction (intensity modeling along Bragg lines) were combined.

References

[1] W. Kuehlbrandt, *Nature* **406** 569-570 (2000).

[2] C. M. Casadei *et al.*, *IUCrJ* **5** 103-117 (2018).