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Revisit the basics to optimize detection systems and time-resolved XAFS

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XAFS has become one of the most important research tools. And it has become easier to take high quality XAFS spectra with the development of many synchrotron facilities. Top-up injection made the synchrotron beam more stable than before.

Needless to say, linear response of the detectors for incoming signal is very important to obtain reliable results. The continuity of XAFS spectra before and after an injection was a good index to check the linearity of the detection systems and stability of the beamline optics. However, it is overlooked by some experimenters. And it is getting difficult to check them with the development of top-up injection. Ionization chamber is one of the most important detectors to measure XAFS. Linearity of ionization chamber can be realized by optimizing the filled gas and electric field. Germanium detector is also a powerful tool to measure fluorescent XAFS of dilute samples. In this case proper deadtime correction [1] is essential. EXAFS signal becomes continuous before and after an injection when the conditions are optimized.

Quick XAFS and dispersive XAFS are two key techniques to measure time-resolved XAFS. Time-resolution of DXAFS is typically milliseconds but it has reached to 100ps by using single-bunch detection. Time required to obtain a quick XAFS spectrum is also becoming milliseconds with the development of some quick scanning techniques. The apparent time-resolutions seem similar but we have to remind that a spectrum is measured simultaneously thus is a time averaged spectrum in the case of DXAFS. But the composition changes during a measurement of a spectrum in case of QXAFS. A simulation will be demonstrated.

[1] M. Nomura, *J. Synchrotron Rad.* **1998**, *5*, 851.

Keywords: DXAFS, quick XAFS, detector

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Development and adoption of scientific data exchange frameworks: a CIF perspective

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In developing a data exchange specification, the XAS community is treading a similar path to that trodden by the developers of the Crystallographic Information Framework (CIF) 20 years ago. Development of the XAS standard specification will benefit from understanding the reasons for the success of CIF in small-molecule crystallography, and conversely the reasons for the less widespread adoption of CIF in other crystallographic fields.

CIF consists of a simple syntax coupled with domain-specific dictionaries developed by experts in the respective fields. The original highly successful CIF effort produced both the syntax and a “core dictionary” for small-molecule crystallography. This core was supported by the IUCr journals, prominent databases, and major software providers. Authors were initially offered faster publication in IUCr journals when presenting publication-ready results in CIF form, and tools were provided that automatically checked CIF files and transformed them into publication-ready PDF files.

Other crystallographic domains (for example powder and macromolecular crystallography) have generally seen much slower adoption of CIF as an exchange format. Reasons appear to include (a) inability to update and/or redistribute legacy software; (b) CIF provides no benefit compared to current practices; (c) lack of broad community support.

The XAS data exchange development process should therefore ensure (a) that widely-used software packages will support the format; (b) that the XAS community is in general agreement with both the goals and the XAS-specific descriptions contained in the specification; and (c) that there is some benefit to be gained from using the new format. Such a benefit could be created by developing and encouraging minimum standards for presentation of XAS data, while providing software that checked conformance to these standards and leveraged the extra metadata to provide new functionality.

Keywords: CIF, XAS, data exchange

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Element selective X-ray imaging of growing chemical patterns

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Chemical pattern formation has been extensively studied because of interesting similarity to patterns on biological systems. Chemical reaction-diffusion systems generates spatial variations in the concentration fields of the reacting chemicals. In the present research, time-spatial distribution of elements have been studied by element selective X-ray imaging using high-flux synchrotron radiation. Though conventional scanning-type X-ray imaging with micro/nano beam has been widely used, the technique requires a long measuring time. To see elements in growing chemical patterns, we have employed novel projection-type X-ray imaging without performing any scans. Some X-ray movies of Tarube's artificial cell and oscillating reactions will be presented.

[1] M. Traube, *Arch. Anat. Physiol. u. wiss. Med.* **1867**, 87-129. [2] K. Sakurai, H. Eba, *Anal. Chem.* **2003**, *75*, 355-359.

Keywords: non-linear system, real time imaging, X-ray fluorescence

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Structural biology of eukaryotic gene transcription

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RNA polymerases are the central multiprotein enzymes that catalyze DNA transcription and RNA synthesis in all cells. Our laboratory uses a combination of X-ray crystallography and electron microscopy to determine the three-dimensional structures of complexes of eukaryotic RNA polymerases with accessory protein factors and nucleic acid substrates. These structures are complemented by functional studies in vitro and in vivo, to obtain mechanistic insights. We have also started to investigate the regulation of gene transcription on a cellular level, by measuring RNA synthesis rates genome-wide.

In my talk I will first summarize our current understanding of the structural basis of gene transcription. I will then concentrate on the