L-24 Friday, 17.06., 9^{00} - 9^{40}

High Brilliance SAXS on synchrotrons

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The brilliance of the X-ray beam is the important quality parameter of X-ray sources. Brilliance sums up the beam parameters such as beam intensity, opening angle of the beam, size of the beam and the proportion of monochromaticity of the X-ray radiation. With existing modern X-ray optics many of these beam parameter can be altered, however beam focusing and the opening angle dependent strongly on the source. Because of the special arrangements of the beamline components SAXS relies on the high brilliance of the X-ray beam delivered by modern synchrotrons. At such state-of-the-art high brilliance beamlines high quality SAXS data are collected within several milliseconds on very small sample volumes. On the other hand, high brilliance X-rays are causing radiation damage especially to biological samples, which has to be treated by counteractions.

New developed, advanced sample environments based on microfluidic devices allows handling sample volumes of several pico-liters. Such devices are used for SAXS high throughput screening of hundreds of different sample conditions. If such a screening campaign includes as well automated data analysis procedures up to final model building, SAXS will be the method of choice for e.g. ligand screening in pharmaceutical industries.

Since microfluidic devices can operate on low flow rates on small channels, effects of low Reynolds numbers provide different types of SAXS experiments. For instance fast mixing of liquids is used for time resolved scattering experiments. Further applications are online sample preparation by applying mechanical and physical stress to the sample. While such techniques allow analyzing the kinetics of chemical or biochemical reactions, need investigations on the dynamics of a system a more sophisticated approach.

At high brilliance X-ray sources classical pump-probe experiments facilitates the analysis of reaction dynamics. For these investigations, for instance an ultra-short laser pulse is triggering the reaction in the sample. The high flux synchrotron beam is used for investigated the structural response of the system. Such experiments need, beside the brilliance of a synchrotron beam suitable fast detector system for recording the data in short time frames.

This lecture introduces the brilliance parameter and describe modern X-ray optics. The fields of applications are discussed and some experimental highlights shown. Possible strategies for handling radiation damage will be presented and future directions of SAXS introduced.

L-25 Friday, 17.06., 9^{40} - 10^{20}

Integration of SAXS with Complementary Techniques for Structural Characterization of Large Biomolecular Complexes

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Structural analysis of multi-domain protein complexes is a key challenge in current biology and a prerequisite for understanding the molecular basis of essential cellular processes. The use of solution techniques is important for characterizing the quaternary arrangements and dynamics of domains and subunits of these complexes. As experimental data for large protein complexes are sparse, it is advantageous to combine these data with additional information from other solution techniques.

In my presentation I will show our recent achievements in integrating Small-Angle X-ray Scattering (SAXS) data with complementary data from Nuclear Magnetic Resonance Spectroscopy, X-ray crystallography, electron microscopy, and mass spectrometry to study structure and dynamics of large disease-related proteins and protein complexes [1-9]. By using our integrated approach we were able to provide a comprehensive and accurate description of protein complex structure and dynamics in a native-like environment. This underscores the central role of SAXS for structure determination of protein complexes and ensures its unique role and contributions in integrated structural biology approaches in the future.

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L-26 **Friday, 17.06., 10^{20} - 11^{00}**

Mineral dust iron geochemistry of the last 160 kyears

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Windblown mineral particles (dust) plays a key role in the climate system and many challenging studies allowed the quantitative estimation of direct and indirect effects on climate and environmental phenomena. Dusts are naturally stored in glaciers and ice sheets from polar areas represent unique natural archives of the particulate present in the atmosphere. Among the many challenging researches on aerosols/dust the current emergency determined by the global warming is triggering scientists to carefully look for signs of past climate changes. Indeed, the reconstruction of past climate trends may be useful to understand the Earth’s climate and, eventually, paleoclimatic data could help to understand the balance between positive feedback components such as greenhouse gases and negative feedback components like mineral dust. The most precise information on Earth’s climate variation can be extracted from ice cores drilled both in polar and mid-latitude-high-altitude glaciers. Within this framework, the characterization of low concentration of airborne particles in natural ice is fundamental. TALDICE (*Talos Dome* Ice Core) is a 1620 m long ice core, retrieved from *Talos Dome*, a peripheral dome of the *East Antarctic* plateau. The proximity to the sea influences the moisture budget and guarantees a high snow accumulation rate and thus a high time resolution of the climatic record. The TALDICE atmospheric dust record presents peculiar features, related to the influence of local *Antarctic* dust sources and to the regional atmospheric circulation, which affects the *Ross Sea* region [1,2].

The reconstruction of undisturbed stratigraphic sequences of dusty ice layers from shallow and deep ice cores provides information on the temporal variability of atmospheric dust loads and allows investigating the dust-climate coupling on different timescales. In addition, characterization of dust dispersed in the ice cores to correlate past environmental and climatic conditions with particles source areas is now possible. Cutting-edge synchrotron radiation-based spectroscopic techniques such as Total-Reflection X-Ray Fluorescence (TXRF) and X-ray Absorption Near Edge Structure (XANES) have been used to investigate in a non-destructive way the microparticle mineralogy. However, experiments are extremely challenging for *Antarctic* ice core samples, where mineral concentrations are extremely reduced and dust is often mixed with poorly crystalline material such as volcanic glasses. Experiments performed at the *Stanford Synchrotron Radiation Laboratory* (SSRL) and at the *Diamond* facility in *Oxford*, allowed to identify and to compare the mineral composition. XANES spectra combined with TXRF results not only demonstrate the feasibility of such kind of analysis but also that it may usefully complement other techniques commonly used in the ice core analysis [3,4].

I will show that the application of techniques usually applied in the field of materials science, mineralogy and crystallography can give an important contribution to ice core science, with new and original information. The interpretation of data and the extraction of useful climatic proxy is still in progress but premises are extremely encouraging. Preliminary results point out that the atmospheric dust deposited at *Talos Dome* during the last 160 kyr is not uniform, pointing out a clear and significant variability. The analysis could be a first step toward the comprehension of this and other unsolved climatic issues.

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