Commercial Lectures

CL1

THE PLANET. PORTABLE HIGH-RESOLUTION POWDER DIFFRACTION

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The Planet is the new portable high-resolution X-ray powder diffractometer from xplorex. The system is based on a modified Seemann Bohlin geometry. This geometry was chosen, because it yields a good resolution while the system can be kept compact.

In this lecture, I will introduce the Planet, discuss the principles of Seemann-Bohlin and how we realized it. We will demonstrate the accuracy of the peak positions as well as the attainable resolution with measurements on LaB_6 and Si. We will conclude with a few examples, where we used the planet for phase identification.

CL2

TECHNICAL SPECIFICATIONS AND YOUR DATA: READING THE LINES AND BETWEEN THE LINES

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The past ten years have seen tremendous advances and progress in X-ray detector technology available for crystallography. Hybrid Photon Counting (HPC) detectors have brought crystallography the advantages of single-photon counting and direct detection in a silicon solid-state sensor. The absence of readout noise and detector dark signal ensure high data quality irrespective of exposure time or number of acquired frames; a digital counter in each pixel enables highest dynamic range and allows the collection of low- and high-resolution data simultaneously. Direct detection of X-rays in solid-state sensors provides a small, sharp point-spread function, a critical advantage for accurately measuring closely spaced reflections or diffuse scattering. Last but not least, direct detection with CdTe as a sensor material provides more than 90% quantum efficiency and makes best use of the precious photons from high-energy sources.

This presentation will give an overview of how HPC technology works and why it provides a number of unique advantages. Furthermore, some highlights from synchrotron and laboratory diffraction experiments will demonstrate how HPC detectors facilitate contemporary crystallography.

CL5

STRUCTURE ANALYSIS OF DRUG DELIVERY SYSTEMS WITH SAXS IN THE LABORATORY

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Small-Angle X-ray Scattering (SAXS) draws increasing attention in the field of pharmaceutical engineering. SAXS is a versatile technique used for shape and size characterization of nanostructured materials between 1 nm and 200 nm. Biological samples, like proteins or viruses are already well known to be investigated with SAXS. Furthermore drug delivery systems like drug loaded vesicles (see example in figure 1), where size and shape parameters of the vesicle and the drug are found or granulate powders, where the internal surface obtained by SAXS correlates with the tablet hardness, are interesting examples of applications in pharmaceutical research.

In this contribution we present select applications of biological samples, employing a multifunctional laboratory Small and Wide Angle X-ray Scattering (SWAXS) system, the SAXSpoint. The SAXSpoint system enables SAXS and WAXS studies at ambient and non-ambient conditions, GI-SAXS, in-situ tensile SWAXS experiments and satisfies the advanced user with a wide range of dedicated sample stages, full experimental flexibility and highest resolution. The system provides simple operation, short

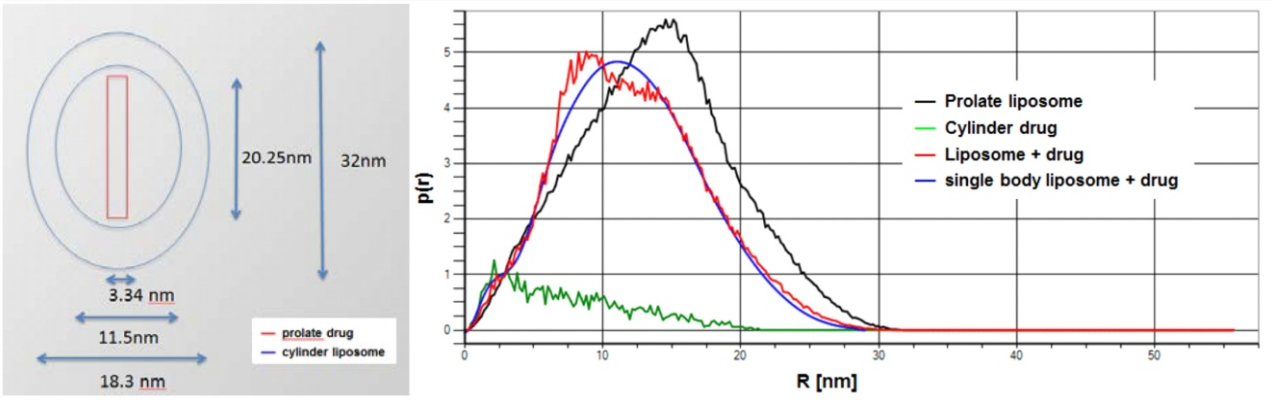

Figure 1. Study of a liposome drug carrier system. Data, obtained from a SAXS-measurement, yielded with aid of single body simulation (simulated Pair Distance Distribution Function on the right side) in the depicted model of the drug-loaded liposome (on the left side).

measurement times and excellent angular resolution, enabled by a smart beam formation concept which includes a brilliant X-ray source, advanced X-ray optics and optimized scatterless collimation while maintaining a laboratory-friendly compact size and small footprint.

Different scattering studies on biological and pharmaceutically relevant samples were performed on the presented SAXSpoint system. Some of the samples required high resolution, i.e. a very low minimum scattering angle in order to resolve large structural dimensions. The unique sample-positioning mechanism enabled WAXS measurements to determine crystallinity without re-aligning any part of the SWAXS system. The presented studies clearly show that high-resolution and high-quality SWAXS data can be obtained with a laboratory SWAXS system.

CL6

PANALYTICAL'S AERIS BENCHTOP POWDER DIFFRACTION SYSTEM

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PANalytical B.V., Almelo, The Netherlands

Aeris is PANalytical's easy-to-operate and user-friendly benchtop X-ray powder diffractometer. With its intuitive operation, Aeris makes X-ray diffraction experiments simple and accessible for everyone. Aeris comes in the editions Cement, Minerals, Metals and Research to address the specific needs of each market. Furthermore, it is the world's first fully automatable benchtop XRD instrument.

Aeris incorporates many technologies that were introduced on our high-end systems and have proven their benefits. The data quality and speed of analysis delivered by Aeris have previously only been seen on full-power systems.

The superior resolution, low angle performance and linearity will be demonstrated by examples of measurements on various materials, such as minerals, catalysts, pharmaceuticals and international standards.

CL7

LATEST DEVELOPMENTS IN LABORATORY SAXS/WAXS INSTRUMENTS

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Xenocs provides complete solutions for characterizing the nanostructure and morphology of materials. The product portfolio of the company includes innovative high performance instruments that combine Small and Wide Angle X-ray Scattering techniques (SAXS/WAXS) for soft matter, nanomaterials, or polymers characterization. Founded as a spinoff company from the Institute Laue Langevin, in Grenoble, France, Xenocs supplies its solutions to leading research and development institutions around the world. On January 2017, Xenocs acquired the Danish company SAXSLAB Aps, recognized leader in high end Small Angle X-ray Scattering laboratory equipment, and its subsidiary SAXSLAB US Inc. based in Northampton, MA, USA.

In parallel to the advent of dedicated synchrotron radiation sources and beamlines, several breakthroughs have been accomplished for laboratory analytical x-ray instrumentation and in particular for Small Angle X-ray Scattering (SAXS) instrumentation. Breakthroughs include X-ray micro-focus sources with aspheric multilayer coated optics, scatterless collimation [1], sample environment, software and hybrid pixel photon counting detectors as well as instrument design with for example multiple source energy capability [2].

Today, these technologies combine to provide in-laboratory SAXS instruments, with a performance comparable to that previously achieved only at synchrotrons. Flexible instrument designs provide simultaneous measurement of Wide Angle X-ray Scattering (WAXS) signal in various sample forms (including thin film) and experimental conditions. The state-of-the-art performance opens the way for a wide range of applications, including scattering from soft matter. Performance and possibilities will be illustrated through a few application examples such as characterization of highly diluted macromolecules or in-situ dynamic studies of complex soft materials.

This presentation will review the latest developments of Xenocs SAXS/WAXS instruments including our new system for biostructural research: the BioXolver.

1. Y.Li et al., *J. Appl. Cryst*., 2008, 41.
2. S. Koppoju et al., *J. Appl. Cryst.*, 2015, 48.

CL8

STOE – TRADITION OF INNOVATION SINCE 1887

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STOE develops, manufactures and sells scientific instruments for the non-destructive analysis of substances. Based on the X-ray diffraction (XRD) method, these systems characterize single crystals and powder samples and give answers to which substances a particular powder or crystal contains or at which positions atoms in solid bodies are exactly located. The majority of customers are institutes at universities and industrial laboratories worldwide doing research in chemistry, pharmacy, mineralogy or material science.

STOE, originally founded in 1887, to manufacture equipment for the optical analysis of crystals, has been a pioneer in powder and single crystal X-ray diffraction since the 1960's, e.g. STOE invented and patented the transmission geometry technique for Powder XRD as well as, for single crystals, produced the first pixel detector XRD system with an open Eulerian cradle.

STOE is based in Darmstadt, Germany, and keeps the R&D, software programming, electrical and mechanical engineering and production all in house, allowing STOE to provide customers with standard as well as individual solutions. Whenever it comes to quality, STOE accepts no compromises. This high-level of detail is what sets STOE apart.

STOE is the partner in X-Ray Diffraction to crystallographers, chemists, material scientists and pharmacists all over the world.