



**Anton Paar**

## SAXSess mc<sup>2</sup>

The Modular Tool for Nanostructure Analysis

::: Innovation in Materials Science



# Experience the Future of Nanomaterials Analysis

Modern materials science and technology goes “nano” – since the presence or implementation of nanostructures in a material can dramatically change its properties. This is true for any kind of material, whether it is inorganic, organic or a composite of both.

Structure formation on the nanometer level is essential for the course of many biological and metabolic processes. In nature, nanostructures build up a huge number of materials with different properties from a relatively small number of basic components. This fact increasingly inspires modern

scientists and represents a huge potential to tailor materials and to influence natural and technical processes. A deeper understanding of the relationship of the material's structure to its physical, chemical and biological properties is crucial in this perspective.

SAXSess mc<sup>2</sup> is the ideal tool to analyze nanostructures present in all different kinds of samples, from liquids (e.g. colloids, protein solutions) to solids (e.g. polymer films, nanocomposites). Its modular design concept allows you to select the optimal setup for your needs in a compact form!





# SAXSess mc<sup>2</sup> Applications - Analyze your Sample of Choice

Modern material research, with its different disciplines, focuses on the nanostructure of various natural and synthetic materials. A precise understanding of the inner arrangement of super-molecular structures ranging from 1 to 200 nm helps the researcher to elucidate the material's properties on the macroscopic scale.

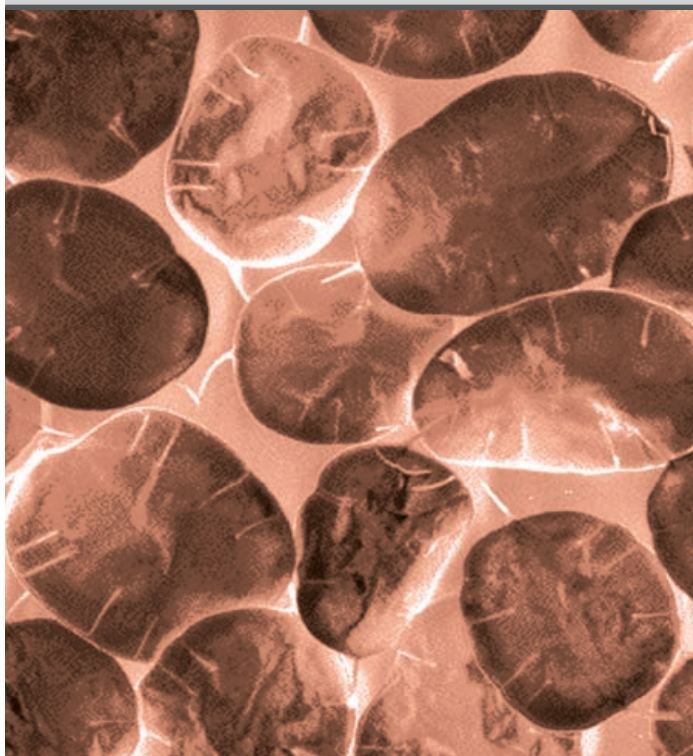
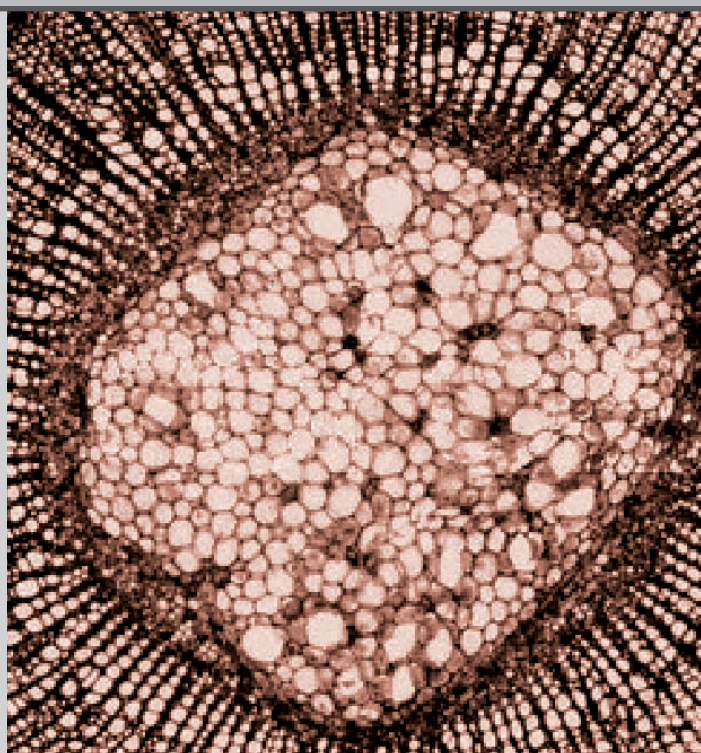
The Small-Angle X-ray Scattering (SAXS) method allows you to obtain information about the morphology of a huge variety of materials, ranging from proteins, nutrients and active pharmaceuticals to polymers, fibers, paints and catalysts.

## Surfactants

Surface-active agents are molecules consisting of two parts, of which one likes to be in an environment of water and the other one likes to be surrounded by oil. Once brought into water (or oil), the surfactant molecules self-assemble and form structures (= micelles or vesicles) which can be spherical, cylindrical or lamellar in shape. Typical samples are detergents, food additives and nutrients, pharmaceuticals and personal-care products.

### SAXSess mc<sup>2</sup> determines:

- ▶ Micelle size
- ▶ Micelle shape
- ▶ Phase behavior
- ▶ Inner structure of vesicle walls

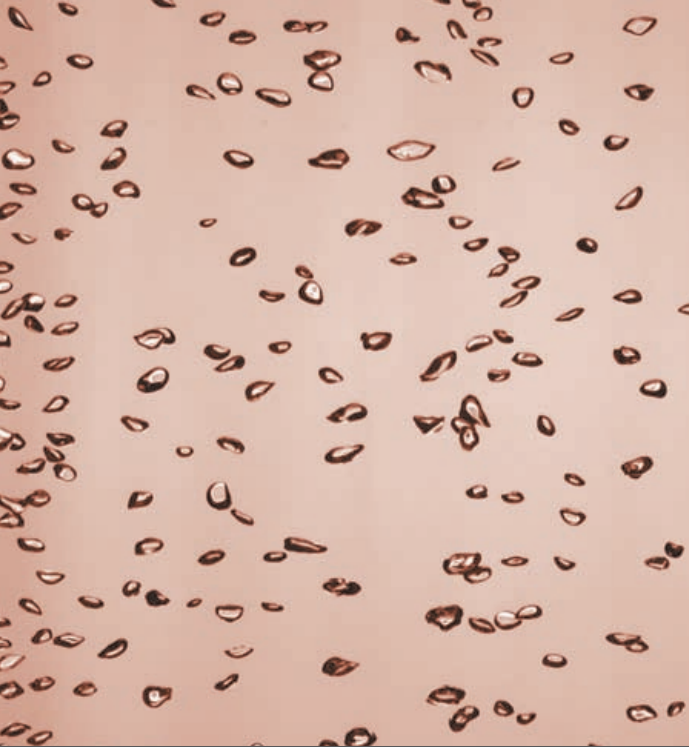


## Biological materials

Information on the structure of proteins, enzymes, allergens and bio-membranes is indispensable for a better understanding of their function in biological processes. SAXS is the method of choice for biomaterials research because investigations can be performed in solution under biological conditions, and structural changes can be studied in vitro.

### SAXSess mc<sup>2</sup> determines:

- ▶ Structural information of proteins in solution (shape, size)
- ▶ Inner structure
- ▶ Aggregation state
- ▶ Molecular weight



## Dispersions

Dispersions are mixtures of particles with liquids (e.g. pigments in paints, inks and sun screens, metal dispersions, blood cells). The particles are stabilized by surface charges or surfactant molecules. Unstable dispersions flocculate due to aggregation by which the particles grow in size until they separate from the liquid. Therefore, the stability of dispersions can easily be observed by determining their size distribution.

### **SAXSess mc<sup>2</sup> determines:**

- ▶ Shape or size distribution of dispersed particles
- ▶ Dispersion stability
- ▶ Particle nucleation
- ▶ Aggregation state

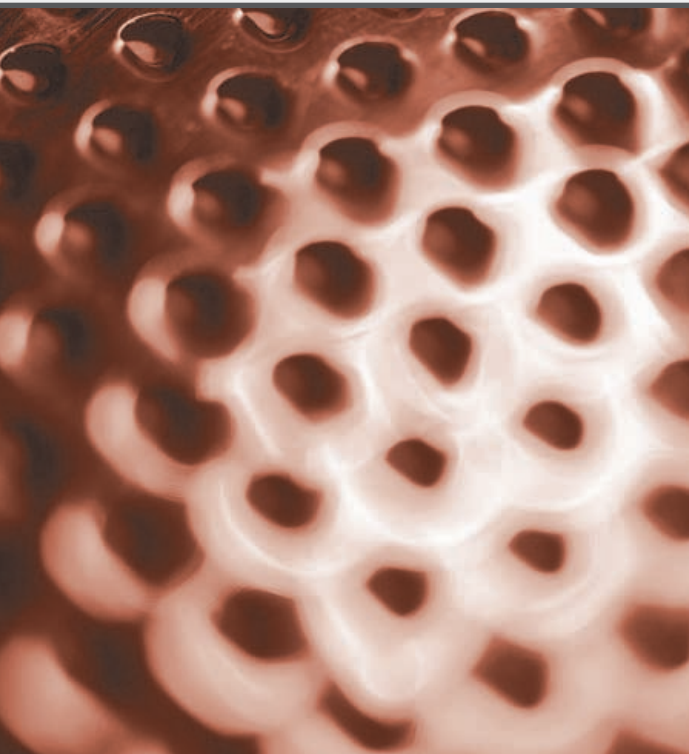
## Fibers

The mechanical, optical or thermal properties of natural and man-made fibers (polymers, composites) can be affected by the manufacturing process. SAXS helps to obtain information on the fiber structure, which is responsible for the fiber's properties.

Thus, fiber production and processing can be monitored and improved.

### **SAXSess mc<sup>2</sup> determines:**

- ▶ Internal structure
- ▶ Crystallinity
- ▶ Specific surface
- ▶ Orientation and orientation distribution



## Catalysts

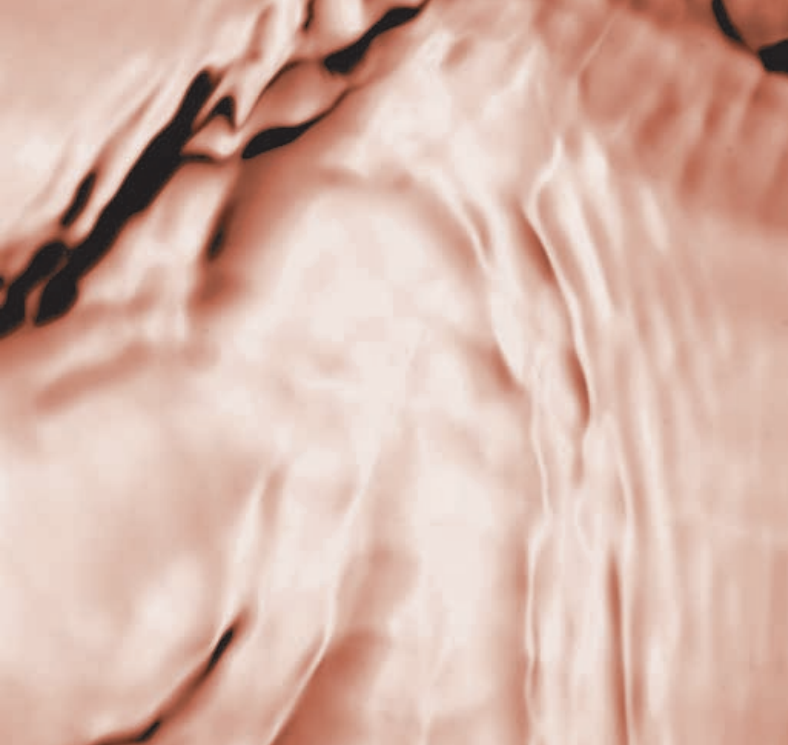
Heterogeneous catalysts consist of small particles or sponges of metal (gold, platinum, etc.) on ceramics with a highly specific surface.

Catalysts are of great importance in a wide field of industrial applications (e.g. petroleum refinement and processing, polymerization, gas purification, fuel cells). Their capability to promote chemical reactions strongly depends on their active surface, which can be determined with the SAXS technique.

### **SAXSess mc<sup>2</sup> determines:**

- ▶ Specific surface (porosity)
- ▶ Particle size
- ▶ Size distribution
- ▶ Crystallinity





## Emulsions

Emulsions are mixtures of two immiscible liquids such as oil dispersed in water (or vice versa). The minor component forms small particles (spheres, cylinders or lamellae) in the major component. These particles are only stable if surfactant molecules cover the interface between the two. Typical samples include food, drug carrier systems, microemulsions and personal-care products.

### **SAXSess mc<sup>2</sup> determines:**

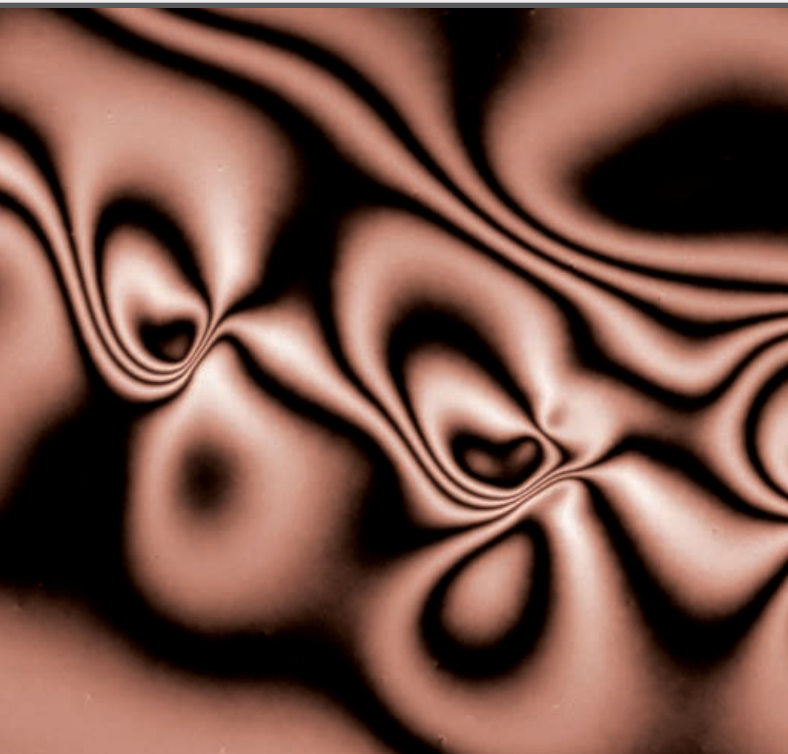
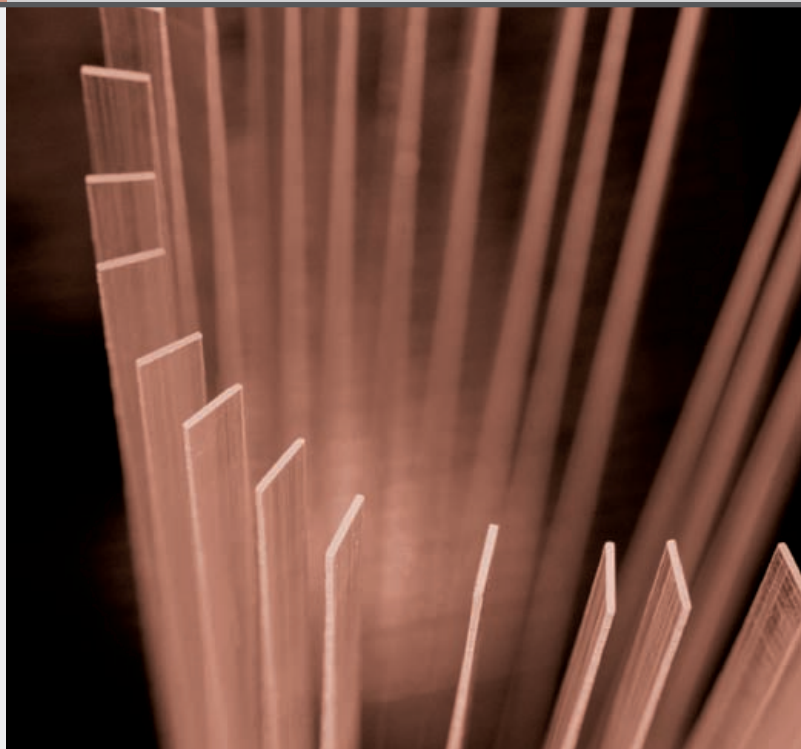
- ▶ Shape and inner structure
- ▶ Size distribution of droplets
- ▶ Emulsion stability at different temperatures
- ▶ Transfer kinetics of encapsulated agents

## Polymers and nanocomposites

Modern polymer research and technology focuses on goal-oriented development of new polymeric materials and improvement of existing products. SAXS can help to study their structure and improve their performance. The types of polymer samples that can be investigated range from semi-crystalline polymers, block copolymers, polymer blends, microemulsions and synthetic fibers to nanocomposites.

### **SAXSess mc<sup>2</sup> determines:**

- ▶ Shape and inner structure
- ▶ Crystallinity
- ▶ Periodic nanostructures
- ▶ Orientation



## Liquid crystals

Liquid crystals are substances that exhibit properties between those of a conventional liquid and those of a solid crystal. Synthetic liquid crystals find wide use in liquid crystal displays (LCDs). Biological liquid-crystalline nanostructures (cell membranes) are abundant in living systems. Many common fluids, e.g. soap, are in fact liquid crystals and form a variety of LC phases depending on their concentration in water.

### **SAXSess mc<sup>2</sup> determines:**

- ▶ Size (distribution) and shape
- ▶ Crystallinity
- ▶ Aggregate ordering
- ▶ Orientation

# Your Insight into Nanostructures

Small-Angle X-Ray Scattering (SAXS) is a well-established analytical method for nanostructure analysis. It is widely used in both scientific material research and routine characterization of materials during production or processing.

The samples are solid or liquid materials which contain nanosized domains of another material. These domains can be solid, liquid or gaseous and range from 1 nm to 200 nm.

When X-rays penetrate such a material they are scattered on the interfaces of the nanostructures. This produces a scattering pattern specific to the structure of the material.

The SAXS method is accurate, economical, non-destructive and usually only requires a minimum of sample preparation. Moreover, SAXS allows you to investigate interactions between molecules in real time. These interactions lead to self-assembly and large-scale structure changes, on which material properties or biological processes often rely.

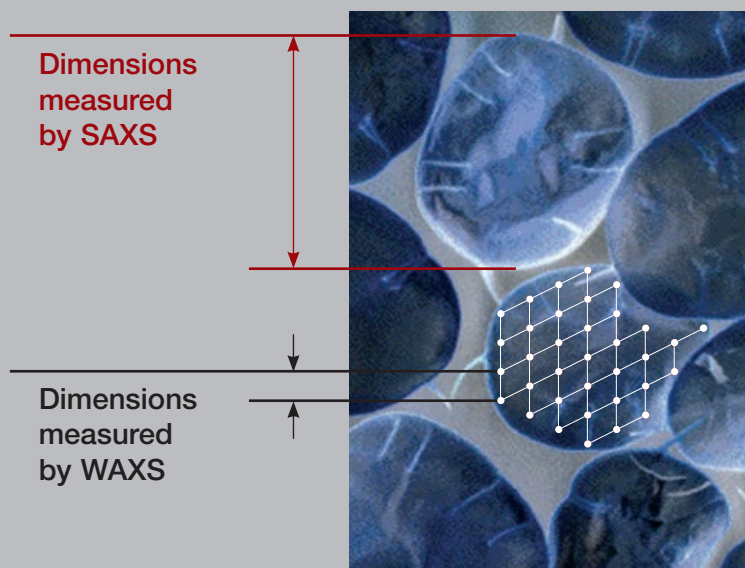
Applications cover various fields from emulsions, liquid crystals and macromolecules to porous materials and metal alloys. They can be found in research and in quality control alike.



## SAXS and WAXS

Nanosized particles and domains scatter towards small angles. The SAXS pattern provides information on their overall size and shape and thus determines the nanostructure of the sample including the orientation of nanodomains.

Atoms and interatomic distances scatter towards large angles. The obtained wide-angle scattering (WAXS) pattern provides information on the phase state and the crystal symmetry.







## Collimation matters

SAXSess mc<sup>2</sup> offers the optimum collimation mode for all types of samples.

### Isotropic samples

Most samples that are investigated by SAXS are isotropic, i.e. they exhibit no preferred or oriented arrangement but are randomly distributed. The optimum experimental mode for these samples is line collimation, offering convincing advantages:

- ▶ Fast measurements at excellent resolution and data quality
- ▶ Superior performance for weakly scattering samples like dilute protein solutions
- ▶ Covering most SAXS applications

### Oriented samples

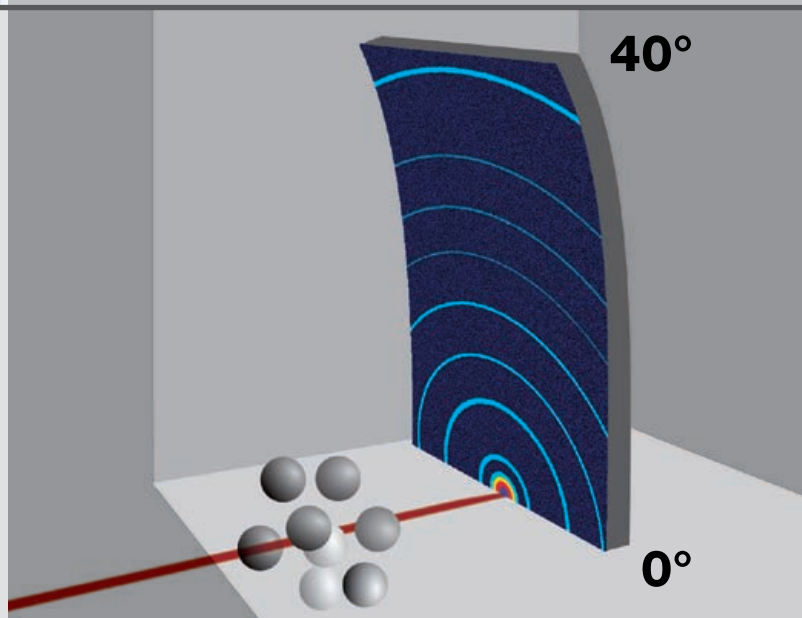
For anisotropic samples exhibiting oriented nanostructures, e.g. sheared or stretched samples, the experimental mode of choice is point collimation:

- ▶ Determination of oriented nanostructures
- ▶ Sample scanning (nanography)
- ▶ Reflectivity (GI-SAXS)

## TrueSWAXS™

The unique TrueSWAXS™ feature of SAXSess mc<sup>2</sup> allows you to measure simultaneously and continuously from small to wide angles (up to  $2\theta=40^\circ$ ), with a consistent high resolution and without changing the instrumental setup.

Therefore, TrueSWAXS™ reveals – in a single run – the complete information on the nanostructure of the sample and its phase state, i.e. whether it is crystalline or amorphous.



# The Benefits

## ▶ All-in-one solution

The fully integrated SAXSess mc<sup>2</sup> combines all components in one system.

## ▶ Modular and compact

The modular SAXSess mc<sup>2</sup> allows you to select the optimal setup for your applications. Due to its compact design SAXSess mc<sup>2</sup> is the smallest laboratory SWAXS system available.

## ▶ Excellent range

SAXSess mc<sup>2</sup> allows you to investigate nanostructures between 0.1 nm and 200 nm.

## ▶ Powerful software

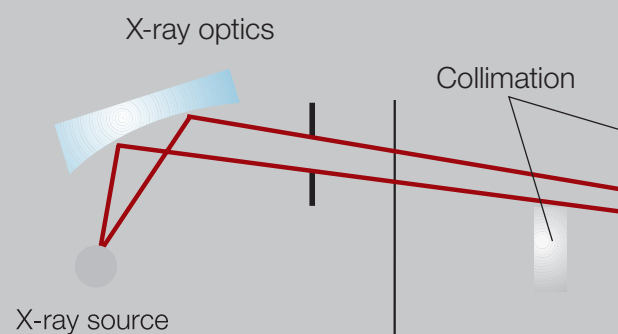
SAXSess mc<sup>2</sup> includes dedicated software for fast data acquisition, data processing and advanced evaluation.

## ▶ Unique TrueSWAXS™

Small- and wide-angle data can be obtained simultaneously and continuously in a single run on the same sample.

## ▶ Easiest-to-use SAXS system

The SAXSess mc<sup>2</sup> design concept ensures easy alignment and speeds up the measurements.





# The Components



## ▶ Powerful X-ray sources

SAXSess mc<sup>2</sup> allows selection of the best suited X-ray source for your application:

- high-speed measurements of isotropic samples or
- studies of oriented samples.

## ▶ Unique X-ray optics

The system provides a highly intense and finely shaped X-ray beam with very low background.

## ▶ Clever sample stages

These make high-throughput screening of liquids and solids as well as multi-directional positioning for sample mapping easily possible.

## ▶ Versatile sample holders

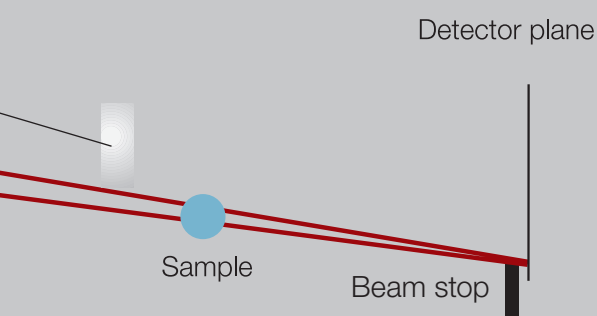
Sample holders can be precisely temperature-controlled and handle virtually any type of sample.

## ▶ High-performance detectors

The SAXSess mc<sup>2</sup> system offers detectors of superior performance for time-resolved and automated SAXS measurements.

## ▶ Peripherals

All peripheral components are included in the SAXSess mc<sup>2</sup> platform.



# Investigate Virtually any Type of Sample

## ASX autosamplers

The ASX autosamplers make high-throughput screening of liquids possible. The measurement and data processing of up to 192 samples can be handled automatically.

For protecting sensitive, e.g. biological samples, while waiting for the measurement, the autosamplers offer a cooling option.

## VarioStage

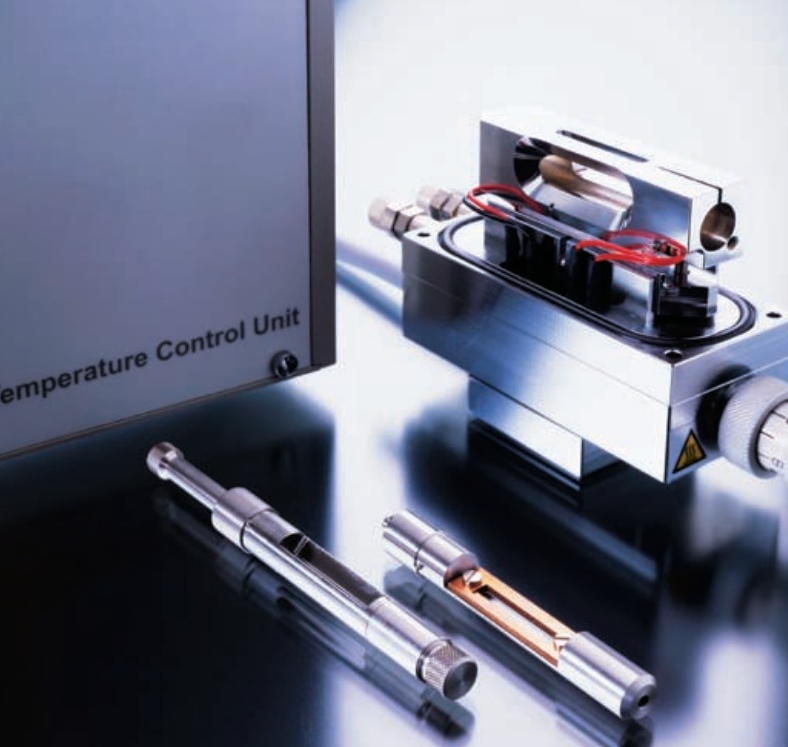
The new multi-purpose VarioStage is applied for screening of solids as well as multi-directional positioning of the sample.

Its precise control of scanning, rotating and tilting the sample is perfectly suited for the investigation of oriented samples. It allows you to perform sample mapping (nanography) and reflection studies.

## High-throughput screening of liquids







## TCS sample stages

The TCS sample stages are used for temperature-controlled measurements of solids and liquids using the dedicated sample holders of the SAXSess mc<sup>2</sup>.

They provide precise temperature control and allow you to perform SWAXS experiments over a large temperature range from -150 °C to 300 °C.

## RotorCell

- ▶ For sedimenting or floating samples
- ▶ For samples with microcrystalline arrangement



## μ-Cell

- ▶ For precious samples (< 10 μl)
- ▶ Full sample recovery after measurement



## Paste Cell

- ▶ For pastes, viscous liquids and powders
- ▶ For samples that need a protective atmosphere
- ▶ SWAXS studies up to 300 °C



## Flow Cell

- ▶ For automated measurements of liquids
- ▶ For reaction monitoring (particle growth, structural changes)



# Dedicated Software - The Essence of a Powerful SAXS System

## SAXSquant™

### Automated data acquisition, processing and analysis

The powerful SAXSquant™ software facilitates data acquisition, processing and analysis.

- ▶ Control of SAXSess mc<sup>2</sup> hardware in order to collect SWAXS data fully automatically.
- ▶ Effective and speedy processing and analysis of SWAXS raw data.

### Device control and automated data acquisition

The SAXSquant™ software controls all system components and allows you to perform automated experiments, including temperature-dependent and time-resolved studies as well as high-throughput screening experiments.

### Fast and simple data processing

SAXSquant™ simplifies data treatment and converts 2D SWAXS images into 1D profiles, which are processed by using fully customizable templates. The software handles large data sets of multiple samples quickly at the push of a button.

### Calculation of particle size and specific volume

SAXSquant™ offers essential evaluation routines such as background subtraction and automatic desmearing. It calculates important sample parameters including:

- ▶ Radius of gyration  $R_G$
- ▶ Particle size
- ▶ Specific volume of a sample

SAXSquant



### Advanced data interpretation and model calculations

#### Particle structure and interaction

The unique PCG software retrieves structural information from experimental SAXS data using mathematical methods (Fourier inversion, deconvolution). Most importantly, these methods are model-free and allow you to determine the particle shape, size and size distribution.

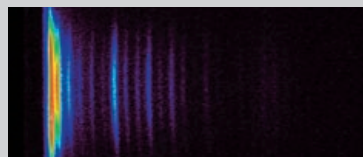
As a unique feature, the software allows you to interpret data of interacting (i.e.





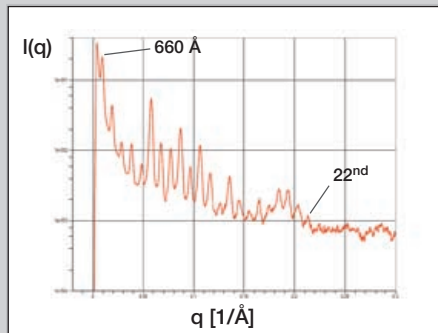
### Automated data acquisition

#### 2D scattering image



### Data processing

#### Background-subtracted 1D curve



*Collagen (chicken tendon), 1 minute*

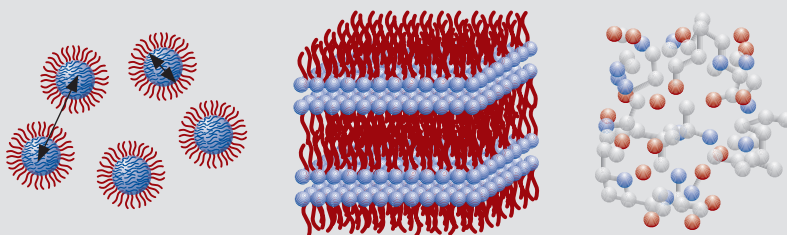
### Data interpretation

#### Model calculations

concentrated or charged) particle systems from a single experiment. It eliminates the need to run a series of measurements at different concentrations and thus speeds up the experiments considerably.

### Simulation and model calculations

In order to relate structure models to the obtained results, the software allows you to design individual structure models or to import crystallographic structure files (e.g. Protein Data Bank files).



# Specifications

<b>X-ray source</b>	Sealed-tube (line and/or point collimation) Microsource
<b>X-ray optics</b>	Focusing graded multilayer optics Advanced line and point collimator
<b>Sample stages / Autosamplers</b>	TCS temperature-controlled stages VarioStage ASX autosamplers for high-throughput screening of liquids
<b>Temperature range</b>	-150 °C ... 300 °C; ± 0.1 °C
<b>Sample holders</b>	Quartz capillaries for liquids Sample holder for solids Paste cell for viscous samples Flow Cell for automation and reaction monitoring µ-Cell for small sample amounts (min. 7µl) Rotor Cell for sample spinning Humidity Cell for powder and film samples
<b>Beam stop</b>	Transparent Precision drive for vertical and tilt alignment
<b>Measuring time</b>	< 1 to 30 minutes (typical)
<b>Detectors</b>	Imaging plate detector (2D data acquisition) CCD detector (2D data acquisition) Others on request
<b>Accessible q-range</b>	$q_{\min}$ : 0.03 nm <sup>-1</sup> and $q_{\max}$ : 28 nm <sup>-1</sup> 200 nm > d > 0.1 nm
<b>Dimensions</b>	Footprint: 1.1 m x 1.8 m
<b>Software</b>	SAXSquant™ data acquisition & analysis software Advanced data interpretation software (PCG)



# Putting the Customer First

## A "one-stop" supplier

At Anton Paar we have everything under one roof: a modern production facility and a versatile R&D department. All SAXSess mc<sup>2</sup> hardware components are developed and produced in-house. Software development is also done in-house and by our cooperation partners in academia.

Our customers receive integral solutions consisting of high-performance hardware and powerful software.

## Our application knowledge – your benefit

We are happy to provide you with profound application knowledge in the field of small- and wide-angle X-ray scattering (SWAXS). Our application specialists continuously work on new applications and share their know-how in a vast collection of

application notes and an extensive guide to SAXS. Thorough user trainings guarantee that you can get started with the SAXSess mc<sup>2</sup> immediately and can benefit from its performance.

Regular workshops and online support for dedicated application questions make sure that we maintain long-term support for our customers.

## Professional after-sales service

Anton Paar has a sales and service network with trained engineers all over the world to provide you with professional after-sales support.

The SAXSess mc<sup>2</sup> small- and wide-angle X-ray scattering system is a high-precision tool. To guarantee its full functionality over a long term, we offer service contracts that provide thorough check-ups on a regular basis.

## Our international sales network



■ Countries with sales representatives

■ Direct sales via Anton Paar GmbH

● Exact location of sales representative



Photos: Croce & Wir, O.D. Lavrentovich, Kent State University



## Anton Paar

**Anton Paar**<sup>®</sup> GmbH  
Anton-Paar-Str. 20  
A-8054 Graz  
Austria - Europe  
Tel: +43 (0)316 257-0  
Fax: +43 (0)316 257-257  
E-mail: [info@anton-paar.com](mailto:info@anton-paar.com)  
Web: [www.anton-paar.com](http://www.anton-paar.com)

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measurement

Rheometry & viscometry

Sample Preparation

Microwave synthesis

Colloid science

X-ray structure analysis

Refractometry

Polarimetry

High-precision temperature  
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