Soft Matter in the Light of Modern X-ray Sources

XV. Research Course on X-Ray Sciences
2-4 March 2016, DESY Hamburg

- Molecular and colloidal glass formation
- Colloidal crystals
- Modern lightsources for Soft Matter characterization
- Structure formation in polymer systems
- Soft Matter surface and interfaces
- Complex fluids

BOOK OF ABSTRACTS

POSTER LIST

Speakers:
V. Abetz (U Hamburg), L. Janssen (U Düsseldorf), A. Pearson (CUI, CFEL), J. S. Pedersen (U Aarhus), A. Petoukhov (U Uetrecht), J. Russo (U Tokyo), B. Ruta (ESRF, Grenoble), F. Schreiber (U Tübingen), M. A. Schroer (DESY), A. Sepe (U Fribourg), M. Sprung (DESY), M. Tolan (TU Dortmund)

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DESY

XV. DESY Research Course 2016 – Soft Matter in the Light of Modern X-ray Sources

Schedule

Wed March 2			
	10:00	Registration	
	10:45	Welcome	
	11:00	**SAXS in Biophysics: Protein-fatty acid and protein-detergent complexes**	Pedersen
	12:00	**lunch**	
	14:00	**Colloidal crystals: going microradian and the role of coherence**	Petukhov
	15:00	**Cracking the glass transition: understanding glassy dynamics from first principles**	Janssen
	16:00	*coffee break*	
	16:30	*facility visits*	
	18:00	**Poster Session**	
Thu March 3	09:00	**X-ray methods to study biological soft condensed matter**	Pearson
	10:00	*coffee break*	
	10:30	**X-ray reflectivity from soft-matter interfaces**	Tolan
	11:30	**Real-time studies of soft matter using X-rays**	Schreiber
	12:30	*lunch break*	
	14:00	**Block Copolymers: Structures in Bulk, Films and Solutions**	Abetz
	15:00	**Nanoscale structural study of soft matter using X-ray scattering**	Sepe
	16:00	*coffee break*	
	16:30	**Crystallization in Soft Matter: a selection of open problems**	Russo
	19:00	*dinner*	
Fri March 4	09:00	**Soft Matter investigated with X-ray Photon Correlation Spectroscopy**	Sprung
	10:00	*coffee break*	
	10:30	**Relaxation processes in complex systems studied with coherent X-rays**	Ruta
	11:30	**Studying orientational order in soft matter systems with X-ray cross-correlation analysis**	Schroer
	12:30	*closure*	

General information

Oral sessions The oral sessions will be held in the FLASH seminar room (Bldg. 28c).

Poster session The poster session will take place in the lobby of the FLASH seminar room on Wednesday 19:00. There will be food and drinks for all participants.

Registration The registration will start on Wednesday 2 March 2016 at 10:00 in the lobby of the seminar room.

Social event The conference dinner will take place on Thursday 3 March 2016 at 19:00 at the DESY canteen.

Meals

Breakfast
If you stay at the Mercure Hotel "Hamburg am Volkspark", breakfast will be provided there. If you stay at the DESY guest house you may have breakfast at the DESY cafeteria (opens at 07:00, building 9) at your own expenses.

Lunch
You may have lunch at the DESY canteen (building 9) and/or the Café CFEL (building 99) at your own expenses.

Dinner
For the poster session we will serve light dinner. On Thursday, 3 March we will have the conference dinner (see above).

Supermarkets LIDL: From the main gate at Notkestrasse turn right and follow the street (700–800m).

PENNY: From the main gate at Notkestrasse walk straight down the street "Zum Hünengrab".

ATM You will find a cash machine in the foyer of the DESY canteen (Bldg. 9).

DESY WLAN An eduroam network is available on the DESY campus.

Guests without eduroam access will be mapped to our "Guest WLAN", it is a DESY Class-C Network which provides DHCP-Support. Before you will get internet access, you have to open your Internet browser with any requested Internet Site. Your request will be redirected to our Portal Server, a DESY form opens automatically. There you have to fill out the required fields. After submitting this form it will take about 1 minute before your requested Internet Site appears. Up to now you can use the Internet connectivity for a maximum of 90 days. **Note:** *The DESY-Guest WLAN is* ***unencrypted****. That means, for transferring sensitive data (e.g. passwords) secure protocols are mandatory (e.g. SSH and VPN).*

Abstracts

SAXS in Biophysics: Protein-fatty acid and protein-detergent complexes

Jan Skov Pedersen

Department of Chemistry and Interdisciplinary Nanoscience Center (iNANO), Aarhus University

Amphiphilic molecules, like surfactant, detergents and fatty acids, spontaneously self-assemble in contact with water and form micelle-like aggregates. Although fatty acids only form globular micelles at rather extreme pH values, they can in contact with proteins form complexes where the fatty acids are organized in a micelle-like structure and the protein in a partly unfolded state decorating the micelle. Such complexes (also termed liprotides) have recently attracted a lot of attention due to their cytotoxicity and their potential for killing cancer cells. We have shown that he structure is quite generic and forms for many different proteins [1]. Ionic surfactants like Sodium Dodecyl Sulfate (SDS) have strong interactions with proteins and similar structures to those of the liprotides forms [2] with the protein in a partly unfolded state. Mixtures of nonionic and ionic surfactants might not interact with the proteins and leave them in a near-native fold [3] and the addition of nonionic surfactants to proteins denatured by ionic surfactants might even make them refold [4]. In fact nonionic surfactants are so gentle to most proteins that they can be used for solubilizing membrane proteins replacing the lipid membrane by a rim of surfactants [5].

In this lecture I will give several examples of application of SAXS in the study of protein-fatty acid and protein-detergent complexes based on the work described in the references. I will also give a bit of background for the SAXS technique and the modelling tools used for extracting the structural information.

[1] Kaspersen JD, Pedersen JN, Hansted JG, Nielsen SB, Sakthivel S, Wilhelm K, Nemashkalova EL, Permyakov SE, Permyakov EA, Pinto Oliveira CL, Morozova-Roche LA, Otzen DE, Pedersen JS. Generic structures of cytotoxic liprotides: nano-sized complexes with oleic acid cores and shells of disordered proteins. Chembiochem. 2014, 15(18):2693-702.

[2] Andersen KK, Oliveira CLP, Larsen KL, Poulsen FM, Callisen TH, Westh P, Pedersen JS, Otzen DE. The Role of Decorated SDS Micelles in Sub-CMC Protein Denaturation and Association. Journal of Molecular Biology 2009, 391(1), 207-226.

[3] Würtz A, Callisen TH, Pedersen JS (unpublished).

[4] Søndergaard A, Kaspersen JK, Otzen DA, Pedersen JS (Unpublished).

[5] Kaspersen JD, Jessen CM, Vad BS, Sorensen ES, Andersen KK, Glasius M, Oliveira CLP, Otzen DE, Pedersen JS. Low-Resolution Structures of OmpA-DDM Protein-Detergent Complexes. ChemBioChem 2014. 15(14), 2113-2124.

Colloidal crystals: going microradian and the role of coherence

Andrei V. Petukhov

Van't Hoff laboratory for physical and colloid chemistry, Debye institute for nanomaterials science, Utrecht University, Netherlands

Application of x-ray scattering to study the self-assembly of colloids is challenging due to the enormous, up to 4 orders of magnitude, difference between the structure period and the x-ray wavelength resulting in very small diffraction angles. Moreover, the intrinsic width of the diffraction peaks possesses information about the long-range positional order. To resolve it, one has to make sure that x-ray waves, which are scattered by particles many lattice periods away from each other, are still able to interfere at the detector. In other words, beam coherence is crucial for high resolution [1]. Various strategies of achieving microradian resolution in small-angle scattering experiments will be discussed.

The results will be illustrated by a couple of examples. In particular, rhombic crystals spontaneously formed by cubic colloids with rounded corners will be discussed [2,3]. Another example will be the dipole-dipole interaction induced transition to a lower-symmetry body-centred tetragonal structure in a system of magnetic core-shell spherical colloids [4].

[1] A.V. Petukhov et al., Current Opinion in Colloid and Interface Science 20, 272-281 (2015). [2] J.-M. Meijer, PhD thesis, Utrecht university, 2015; J.-M. Meijer et al., to be published. [3] J.-M. Meijer et al., Soft Matter 9, 10729-10738 (2013). [4] A. Pal et al., Angew. Chem. Int. Ed. 54 (2015) 1803.

Cracking the glass transition: understanding glassy dynamics from first principles

Liesbeth M.C. Janssen

University of Düsseldorf

The liquid-to-glass transition remains one of the deepest unsolved problems in condensed matter science. Although a wide diversity of theoretical views has been developed to describe this phenomenon, there is still no general consensus on the physical mechanisms underlying the transition. In this talk, I will first give a general introduction to the topic, and then present a novel theory of glass formation, referred to as generalized mode-coupling theory (GMCT), that can potentially shed new light on complex glassy phenomena. GMCT is based entirely on first principles, seeking to predict the full time- and temperature-dependent dynamics of glass-forming systems using only static structural information as input. Ultimately, this work can help to elucidate the intricate link between structure and dynamics in disordered matter, and may pave the way toward a rigorous microscopic understanding of the glass transition.

X-ray methods to study biological soft condensed matter

Arwen Pearson

The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

I will discuss the use of X-ray crystallography and scattering to study biological macromolecular structure, with an emphasis on the practical aspects of sample preparation, handling, data acquisition and analysis. I will also cover more advanced data collection methods to probe dynamic processes such as enzyme reactions or conformational changes.

X-ray reflectivity from soft-matter interfaces

Metin Tolan

Fakultät Physik & DELTA, Technische Universität Dortmund, Germany

The properties of soft-matter thin films (e.g. liquid films, polymer coatings, Langmuir-Blodgett multilayers, protein films) nowadays play an important role in materials science. They are also very exciting with respect to fundamental questions: When liquids and polymers form thin films, they may be considered as trapped in a quasi-two-dimensional geometry. This confined geometry is expected to alter the properties and structures of these materials considerably. This talk is dedicated to the scattering of x-rays by soft-matter interfaces. X-ray scattering under grazing angles is the only tool for investigating these materials on atomic and mesoscopic length scales. A review of the field is presented with many examples.

Real-time studies of soft matter using X-rays

Frank Schreiber

University Tübingen

Functional organic materials and devices are becoming increasingly complex. Their preparation and growth is, not surprisingly, similarly complex, and the resulting structure will be determined by a competition between kinetics and thermodynamics, which is not trivial to predict in particular for multi-component systems. This makes careful and detailed experiments on the structure evolution mandatory. X-ray scattering is ideally suited for studying the structure in situ in a non-invasive way. It can even be applied in real time, which is a key advantage for transient structures and other typical non-equilibrium effects occurring during growth.

In this lecture, we discuss general concepts [1] and recent examples [2,3] of organics-based heterostructure growth in the context of kinetic effects compared to thermodynamic (equilibrium) structure. These include unconventional roughening and smoothing behavior at interfaces as well as unconventional structural motifs, such as a frozen-smectic structure formed in a blend of organic semiconductors which form conventional crystals as pure compounds [4]. Particular attention is paid to the case of kinetically limited phase separation of a donor-acceptor pair (DIP:C60) used in organic photovoltaics [5]. This leads to asymmetric domain sizes near bottom vs. top electrode due to the time (thickness) dependent phase separation with important implications for device modeling [1,6]. We also discuss the associated optical properties and the question of coupling between donor and acceptor components [7,8]. Finally, we comment on the implications of the structure and morphology for the optical and electronic properties as well as possible device applications with focus on organic photovoltaics [1,6].

Contributions by A. Hinderhofer, C. Frank, K. Broch, F. Anger, J. Novak, R. Banerjee, A. Gerlach, and S. Kowarik, are gratefully acknowledged.

[1] A. Hinderhofer and F. Schreiber, ChemPhysChem, 13 (2012) 628. A. Dürr et al., Phys. Rev. Lett. 90 (2003) 016104. S. Kowarik et al., Phys. Rev. Lett. 96 (2006) 125504. S. Bommel et al., Nature Comm. 5 (2014) 5388.

[2] A. Hinderhofer et al., J. Phys. Chem. C 115 (2011) 16155.

[3] A. Hinderhofer et al., J. Chem. Phys. 134 (2011) 104702.

[4] A. Aufderheide et al., Phys. Rev. Lett. 109 (2012) 156102.

[5] R. Banerjee et al., Phys. Rev. Lett. (2013).

[6] J. Wagner et al., Adv. Funct. Mater. 20 (2010) 4295.

[7] K. Broch et al., Phys. Rev. B 83 (2011) 245307.

[8] F. Anger et al., J. Chem. Phys. 136 (2012) 054701.

Block Copolymers: Structures in Bulk, Films and Solutions

Volker Abetz

University of Hamburg, Germany

After an introduction about the potential of block copolymers in different application areas the lecture will cover some thermodynamic basics of block copolymer self-assembly and their self-assembled structures mainly in the bulk state, but also in films and solutions will be discussed. The material will be discussed on the basis of results which are obtained by analytical tools like small angle X-ray scattering and mostly electron microscopic techniques.

References:

7.02 - Block Copolymers in the Condensed State
Adriana Boschetti-de-Fierro, Volker Abetz. *Polymer Science: A Comprehensive Reference* **7** (Nanostructured Polymer Materials and Thin Films) 3-44 (2012)

Janus Micelles
Rainer Erhardt, Alexander Böker, Heiko Zettl, Håkon Kaya, Wim Pyckhout-Hintzen, Georg Krausch, Volker Abetz, Axel H. E. Müller. *Macromolecules* **34**, 1069-1075 (2001)

Morphology, dynamic mechanical properties, and phase behavior of ABC-triblock copolymers with two semicompatible elastomer blocks
Claudius Neumann, D. R. Loveday, Volker Abetz, Reimund Stadler. *Macromolecules* **31**, 2493-2500 (1998)

Nanoscale structural study of soft matter using X-ray scattering

Alessandro Sepe

Adolphe Merkle Institute, University of Fribourg, Switzerland

The structural characterisation of novel organic materials is of great importance for the development of new organic electronic technologies, such as organic photovoltaics (OPVs) and organic field effect transistors (OFETs). Conventionally, blending together a donor (p-type) and an acceptor (n-type) material forms the functional layer, the morphology of which is of great importance. An interpenetrating network on the nanometre scale with a large interface between both the materials is thought to be optimal for organic electronic applications. Structure formation of organic materials is dominated by the morphology of the blended materials, the understanding of which is important as their interplay mechanism can be influenced through the device manufacture protocol. A fundamental understanding on the structural properties of the nanocomposite organic materials is thus indispensable for the further development of the corresponding organic and hybrid electronic devices. Therefore organic nanocomposites are investigated through structural studies employing a broad range of advanced X-ray scattering methods, thus laying the scientific groundwork for a wide range of organic devices and the development of more efficient and environment friendly organic electronics.

Crystallization in Soft Matter: a selection of open problems

John Russo

University of Tokyo

The last decade has seen a flourishing of studies on the crystallization of important Soft Matter systems. The accessible time and length scales that Soft Matter uniquely provides, has in fact allowed to access the early stages of the crystallization process, unveiling its microscopic pathway. In this Lecture we will review some recent theoretic and simulation developments, focusing on open problems that will soon be within reach of experimental investigation. We will review our fundamental understanding of nucleation in the simplest soft matter system, i. e. the hard sphere fluid, and then move to more complicated system, where we highlight the role that directional interactions can have in designing new materials with unique and desirable properties.

Soft Matter investigated with X-Ray Photon Correlation Spectroscopy

Michael Sprung

DESY, Hamburg, Germany

Compared to previously existing X-Ray sources, 3rd generation synchrotron storage rings offer a tremendous gain in brightness. This technological improvement made it feasible to produce partially coherent X-ray beams for the first time and led to the development of coherent X-Ray scattering techniques like e.g. X-Ray Photon Correlation Spectroscopy (XPCS). XPCS is the X-Ray analogue of Dynamic Light Scattering (DLS) in the visible light regime and investigates slow dynamical processes on small length scales. This presentation will introduce XPCS and demonstrate its possibilities to study soft matter problems by discussing a few selected examples.

Relaxation processes in complex systems studied with coherent X-rays

Beatrice Ruta

ESRF, Grenoble, France

A large class of materials, ranging from glasses to soft matter and biological systems, undergo structural arrest and physical aging [1]. Following different experimental routes, like decreasing the temperature in a glass former liquid or increasing the packing fraction in a colloidal suspension, these materials can be driven in an out-of-equilibrium state, where their properties depend on the previous history of the system and spontaneously evolve with time. This process leads to an extremely complex dynamical scenario, characterized by a dramatic increase of the structural relaxation time and the emerging of multiple relaxation processes.

The slow dynamics of out-of-equilibrium materials can be followed thanks to the unique properties of X-ray Photon Correlation Spectroscopy which probes the dynamics at the nanometric [2] and atomic scale [3]. Here I will show several examples on the relaxation processes occurring in arrested states, including bi-dimensional gels, concentrated colloidal suspensions and structural glasses.

[1] P.G. Debenedetti and F.H. Stillinger, Nature 410, 259 2001; L. Cipelletti, et al., Faraday Discuss. 123, 237, 2003.

[2] D. Orsi et al. Scientific Rep. 5, 17930, 2015; R. Angelini et al. Nature Commun. 5, 4049, 2014.

[3] V.M. Giordano and B. Ruta, Nature Commun. 7, 10344, 2016; Z. Evenson et al. Phys. Rev. Lett. 115, 175701, 2015.

Studying orientational order in soft matter systems with X-ray cross-correlation analysis

Martin A. Schroer

DESY, Hamburg, Germany

X-ray scattering methods are perfectly suited to study soft matter systems and allow to determine the structure and phase transitions with high spatial resolution. Standard measurements, however, mostly access spatially averaged information, thus not yielding insights into the samples' local orientational order. For soft matter samples, in particular, the transition from ordered to disordered states can be induced easily and can have significant effects on their properties. In my lecture, I will introduce the concept of X-ray cross-correlation analysis (XCCA) to study the orientational order. The possibilities of this technique to study soft matter study, like colloidal thin films and colloidal crystallites, will be demonstrated.

List of posters

Poster session

No.	Name	Title
1	Abdullah, Malik Muhammad	An approach to calculate the scattering intensity from nanocrystals using hard x-ray beams
2	Chang, Baobao	Structural evolution of isotactic polypropylene during creep under sub yield stress: a study by in situ synchrotron small angle X ray scattering
3	Dourki, Ibrahym	Spatial resolution enhancement of fast electron detectors for imaging applications
4	Fischer, Birgit	Magnetic hydrogels: Synthesis and Characterization
5	Geng, Shiyu	Single-step method for producing cellulose based nanocomposites with outstanding dispersion
6	Jain, Avni	Local structure of supercooled water
7	Keller, Thomas	Amphiphilic Nano-Templates based on Double-Crystalline Co-Oligomer Films
8	Korzeb, Karolina	Grazing-incidence small-angle X-ray scattering (GISAXS) study of block copolymer films during solvent annealing
9	Kurta, Ruslan	Local structure of semicrystalline P3HT films probed by nanofocused diffraction
10	Liu, Yingxin	Real-time probing of the cellulose nanocrystal assembly in levitation droplets via in situ small angle X-ray scattering
11	Nack, Annemarie	Hindered nematic alignment of hematite spindles in viscoelastic matrices
12	Sarma, Abhisakh	Tuning the Superionic Transition temperature of Copper(I) Sulphide nanowires
13	Schulz, Florian	Synthesis and Characterization of Polymer Coated Gold Nanoparticles
14	Sheyfer, Dina	Local structures in glass-forming fluids studied by higher-order intensity correlations
15	Svane-Boysen, Bjarke	Heterogeneous load distributions in cortical bone revealed by diffraction tomography
16	Trebbin, Martin	Microfluidics and X-ray Scattering for Time-Resolved Studies In Situ
17	Valerio, Joana	A liquid jet setup for x-ray scattering experiments on complex fluids
18	Zaluzhnyy, Ivan	Direct reconstruction of the pair distribution function in the hexatic liquid crystals from diffraction patterns
19	Ziegert, Falko	Structure and self-diffusion in binary mixtures of charge-stabilized colloidal suspensions
20	Zozulya, Alexey	Temperature-induced evolution of particle shape and lattice strains in colloidal crystals
21	Passow, Christopher	Depolarized light scattering form anisotropic particles: the influence of the particle shape on the field autocorrelation function
22	Burla, Federica	Shaping collagen networks

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