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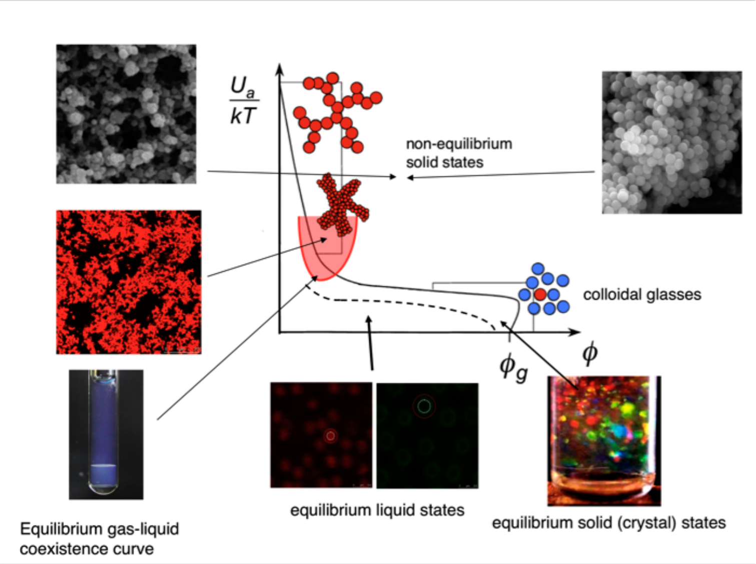

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Société Suisse pour la Diffusion des Neutrons
Swiss Neutron Scattering Society

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5232 Villigen PSI, Switzerland
phone: +41(0)56 310 46 66
fax: +41(0)56 310 32 94
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Bank Account: Postfinance: 50-70723-6 (BIC: POFICHBE)
IBAN: CH39 0900 0000 5007 0723 6

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ON THE COVER:

Schematic state diagram of colloidal particles with short-range attractive interaction potentials, see related article by P. Schurtenberger and Anna Stradner.

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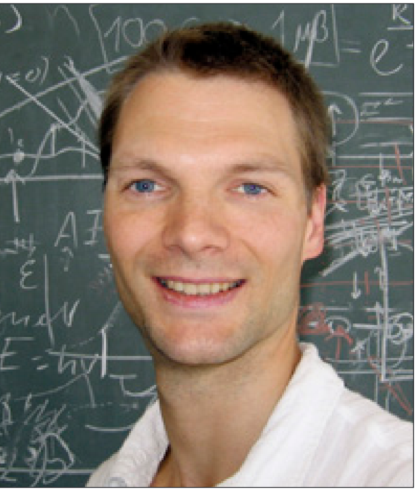

DEAR MEMBERS

The recent meeting of the European Neutron Scattering Association (ENSA) on may 11–11th in Barcelona was interesting. It was my first chance to represent Switzerland as a delegate, but more importantly it was the first meeting with our new chairman Michael Steiner. With the ESS Preparatory Phase project finishing and the ESS site decision, the main focus areas of ENSA in the past years have reached completion. The meeting in Barcelona therefore served to discuss what initiatives and roles ENSA should undertake in the near to medium future.

Two topics were discussed in more detail: education of neutron scatterers, and outreach to new user communities. Obviously, both these aspects will be important once ESS goes online, but already before are they pivotal to a vital neutron scattering community.

There already exist a number of neutron schools – both general 'introduction to neutron scattering', specialized schools focusing on specific aspects, such as biological applications or e.g. electronvolt spectroscopy, and wider topical schools where neutron scattering is taught as an integrated part – e.g. the PSI Summer School on Condensed Matter Research (school.web.psi.ch). ENSA can contribute by spreading knowledge of existing schools, be a forum for coordination of e.g. topics and timing of schools, and assist the creation of new schools. In this context it should be known that within the NMI3 framework program 7 there is support for schools that promote use of neutrons and muons (neutron.neutron-eu.net/n_nmi3fp7/training).

Especially in relation to the prospect of ESS but also for the general future of neutron scattering, is it important to cultivate new fields and users of neutron techniques. It was decided to identify several scientific areas and stimulate the use of neutrons by organizing wider scoped conferences and workshops – in collaboration with neutron facilities. A model example for this approach is the upcoming conference on Neutrons for Global Energy Solutions organized by JCNS, ISIS and ORNL in Bonn September 26-29 (www.congressa.de/NGES-2010).

In this context, we will highly appreciate any input from you – the Swiss neutron scatterers. Do Swiss neutron using laboratories have sufficient access to neutron schools for training their students? Are the school thematics suitable? Are the neutron schools conveniently balanced around the calendar year? Likewise, please forward any ideas and suggestions concerning potential new areas of neutron users, and topics for workshops that could stimulate them.

In an effort to share the knowledge between uses and users of neutron scattering within Switzerland, we will try each time to bring an article from a group or laboratory that uses neutron scattering. In this issue you can enjoy the article by P. Schurtenberger and A. Stradner. Suggestions for groups to be presented in future issues are most welcome.

Concerning Swiss engagement in ESS and ILL (which we could perhaps baptize CHESS and CHILL), I am looking forward to the first contact with the Sate Secretariat for Education and Research (SER). Meanwhile, I wish you all an enjoyable summer and a successful second half of 2010.

Henrik M. Ronnow

Soft Matter – From Model Atoms to Protein Condensation Diseases

Peter Schurtenberger[1] and Anna Stradner

Adolphe Merkle Institute, University of Fribourg, 1723 Marly, Switzerland
[1] Current Address: Physical Chemistry 1, Lund University, S-221 00 Lund, Sweden

INTRODUCTION

Soft condensed matter represents a highly active field of research in which the primary focus is on three different but complementary fields: colloids, polymers and surfactants. However, soft condensed matter science is not only an attractive field in modern basic research, but also of considerable importance in areas as diverse as life, food and materials science and nanotechnology. At the University of Fribourg, we have thus developed during the last 11 years a research program that focuses on fundamental and applied colloid-based soft matter research with the aim of understanding the formation processes, structure, and functional properties of the nanostructured systems that play an important role in various sectors, such as materials and food science. Our research is thus not only driven by scientific curiosity, but we constantly seek to utilize our profound understanding of the equilibrium and non-equilibrium properties of soft matter systems in order to explore new routes towards nanotechnology-based applications. In this overview article we will introduce several key areas of our research activities and demonstrate, how neutrons can be used to explore complex soft matter states in and out of equilibrium. Rather than giving an in-depth description of specific results or a well-balanced state-of-the-art review of the field, we focus on a short summary of some of our activities that were conducted using European neutron sources such as ILL and SINQ. The report covers work that has been conducted during these 11 years in Fribourg, first in the Physics Department, and during the last two and a half years in the Adolphe Merkle Institute.

The properties of colloidal suspensions often combine the features of classical solids and liquids in varying proportions. An important feature of these suspensions is the extremely large range of characteristic length ($0.1–10^4$ nm) and time scales (10^{-9} to 10 sec) that needs to be covered in any attempt to characterize and understand their properties.

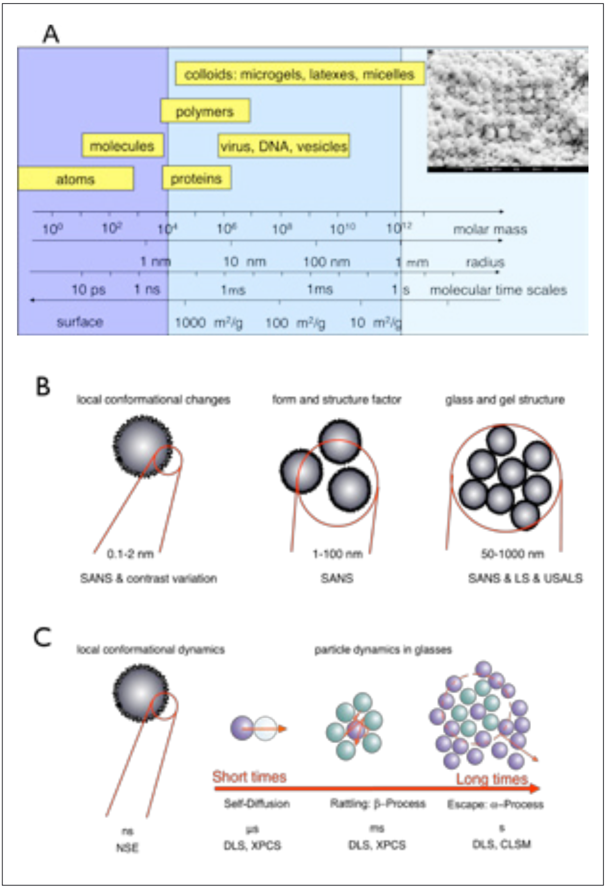

Figure 1:
A) A comparison of the characteristic mass, length and time scales and specific surfaces of complex fluids to those of atomic and macroscopic systems. Note that only time scales required for center of mass diffusion are considered, and local dynamics on molecular scale have not been included.
B) Different characteristic length scales for structural features of sterically stabilized colloids that can undergo a glass or gel transition.
C) Related characteristic time scales for the different dynamical processes that the systems in B) exhibit. Also shown are techniques that can be used to explore these features (SANS: Small-Angle Neutron Scattering; LS: Light Scattering; USALS: Ultra-Small-Angle Light Scattering; NSE: Neutron Spin Echo; DLS: Dynamic Light Scattering; XPCS: X-ray Photon Correlation Spectroscopy; CLSM: Confocal Laser Scanning Microscopy).

This is illustrated in Figure 1A, which compares the characteristic mass, length and time scales (note that only time scales required for center of mass diffusion are considered, and local dynamics on molecular scale has not been included) and specific surfaces of different soft matter systems to those of atomic and macroscopic systems. Figures 1B and C also show the different structural and dynamic features of sterically stabilized colloids, where the polymer layer on the particle surface can induce an attractive interaction between the particles when brought into a poor solvent, and thus induce a liquid-solid transition. Moreover, many interesting features of complex fluids are linked to the existence of non-equilibrium states and closely related to the application of external fields and variable processing conditions, which require the availability of suitable techniques for a non-invasive and in-situ characterization.

The recent progress made in the understanding and application of colloidal suspensions is directly linked to the development of new characterization tools. Among the many experimental techniques used to investigate soft matter, neutron scattering has played a unique and very successful role. There are mainly two reasons why neutron scattering has contributed so much to the advancement of this research field: (i) The suitability of the length and time scales accessed, especially by Small-Angle Neutron Scattering (SANS) and Neutron Spin Echo (NSE). These techniques allow the exploration of large-scale properties (for instance, the structure of colloidal suspensions) as well as features characteristic of the local scales (e.g. the structure of and inter- and intra-chain correlations in a polymer layer). (ii) The capability to manipulate the contrast between the structural units or molecular groups that enables us to study complex systems selectively. In particular, the large contrast achieved by isotopic substitution of Hydrogen (one of the main components of soft matter) by Deuterium constitutes a powerful tool for deciphering complex structures and dynamic processes in these materials. Moreover, the high penetration of neutrons in matter allows the study of the influence of external fields such as applied shear forces or electric and magnetic fields, the influence of confinements and surfaces and in general the evolution of a complex fluid under processing conditions.

However, it is also clear that neutron scattering alone will often not be sufficient for a complete characterization of complex fluids, and additional and complementary techniques will have to be applied in order to probe length and time scales outside the range of neutron scattering. These include for example static (SLS) and dynamic (DLS) light scattering, diffusing wave spectroscopy (DWS), X-ray photon correlation spectroscopy (XPCS) and confocal laser scanning microscopy (CLSM). This is especially important in the investigation of the dynamics of soft matter, where the currently available neutron spectrometers for inelastic and quasielastic scattering experiments are limited to too low values of the accessible relaxation times in particular for colloidal suspensions.

The use of colloids in condensed matter physics has seen an enormous surge of interest due to the fact that colloidal suspensions can conveniently be used as tunable model systems for atomic and molecular systems (Anderson & Lekkerkerker, 2002). They provide new insights into phase behavior and phase transitions because they facilitate experimental observations at quasi-atomic length and time scales. They also allow for a variation of the form, strength and range of the interaction potential almost at will, in contrast to the situation encountered when working with atomic or molecular systems. In our work we have in particular focused on liquid-solid transitions that are often summarized under the headline of dynamical arrest, i.e. transitions that describe the formation of colloidal gels and glasses (Dawson, 2002; Zaccarelli, 2007). Moreover, we have explored the possibility to directly apply the experimental and theoretical framework developed in our colloid physics projects to other fields such as life and food science.

A particularly interesting area, where experimental and theoretical concepts from colloid physics can be applied, is life science. Direct analogies between colloids and globular proteins have helped to advance our understanding of dense protein solutions. The close analogy between the phase behavior of colloids interacting via a short-range attractive potential and globular proteins for example led to a very interesting colloid physics-based approach to rationalize some of the phenomenological observations made during protein crystallization. In our own work, we have focused on the structural and dynamic properties of concentrated protein solutions, and we will show below that neutron scattering has played a very crucial role in these studies.

COLLOIDS AS MODEL ATOMS

Colloidal suspensions have frequently been used as ideal model systems to address fundamental issues in condensed matter physics such as liquid ordering, crystallization and glass formation and the corresponding structural and dynamic properties of the various systems as a function of the interaction potential. With the equilibrium behavior of colloidal systems seemingly well understood, attention recently turned to non-equilibrium phenomena. This already led to fascinating findings that include metastable liquid-liquid phase separation and dynamically arrested states such as attractive and repulsive glasses as well as transient gels. Our current understanding of the different suspension states that occur for colloids with short-ranged attraction as a function of the strength of the attraction and the particle volume fraction is summarized in Figure 2. For ideal hard sphere particles, we observe the formation of colloidal crystals above volume fractions of about 0.49, followed by a transition to a disordered solid phase, a glass, at volume fractions of approximately $\phi \approx 0.58$. If a weak and short-ranged attraction is now turned on, this leads to the astonishing observation of a melting of the glass, followed by a so-called re-entrant glass or solid formation at even stronger attractions.

In the other extreme case of very strong attraction, we reach the regime of so-called irreversible aggregation where one observes the formation of soft fractal gels already at very low volume fractions. The analogy between colloidal glasses at high densities and colloidal gels at low volume fractions has stimulated a considerable effort to explore new ways to characterize, understand and use amorphous solid-like soft matter systems. However, we are still far from having developed a general theoretical framework that is capable of unifying the entire range of concentrations and type of interactions that have been investigated.

At intermediate strength of the attraction, the situation is even more complicated due to the fact that phase separation into a dilute (gas-like) and a concentrated (liquid-like) suspension can occur. The position of the corresponding coexistence curve between the dilute and concentrated suspension can then intersect with the arrest or gel line, and the phase separation can subsequently lead to the formation of a long-lived ‘interaction network’ (a transient gel) of particles, if the attractive interactions between them are strong enough.

Here surface-functionalized organic core-shell particles with a polystyrene core and a polyethylene oxide-based shell can serve as convenient model systems to investigate gela-

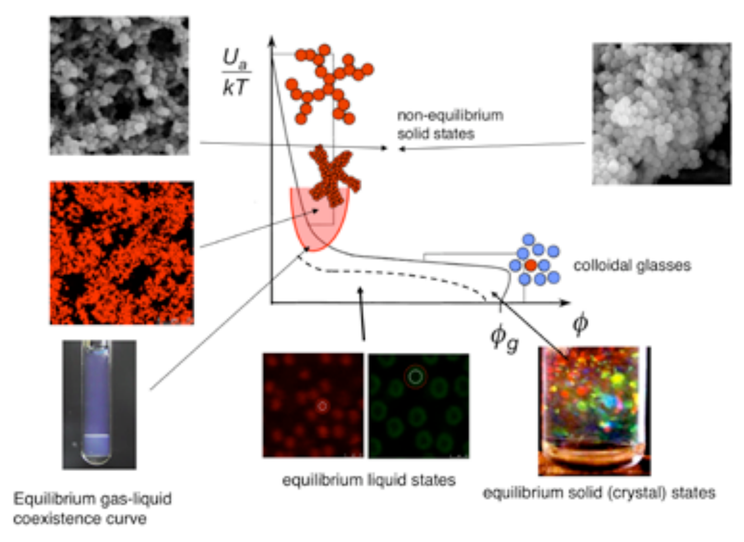

Figure 2: Schematic state diagram of colloidal particles with short-range attractive interaction potentials, where different liquid and solid-like states of colloidal suspensions are plotted as a function of volume fraction Φ and strength of the attraction U_a. The solid line in the energy/composition diagram represents the boundary for the formation of disordered solids, the so-called gel or glass line. The dashed line represents the phase boundary for the liquid-crystal transition. Also shown are several examples from the different regions of this state diagram. The two SEM micrographs shown in the upper right and left part illustrate the close analogy between the structure of dense colloid gels (right, SiO_2 particles) used in sol-gel ceramics production and casein particle gels produced in yoghurt formation (left). The photograph in the lower right corner illustrates the formation of colloidal crystals made from hard spheres that exhibit a colorful appearance due to the existence of Bragg diffraction peaks when illuminated with white light. The two CLSM pictures in the bottom illustrate dense suspensions of fluorescently labeled core-shell particles that allow us to monitor fluid structure and dynamics. Finally, the lower left corner shows examples of either fully phase-separated suspensions, or the appearance of an arrested spinodal decomposition monitored again by CLSM.

tion in short range attractive particle systems. Surface-grafting of polymer on colloidal particle surfaces represents a highly effective means of stabilizing colloidal particles. However, on worsening solvent conditions even such sterically stabilized colloids aggregate. Provided that the grafting density is sufficiently high, aggregation can be maintained fully reversible. This is illustrated schematically in Figure 3A. Thus, sterically stabilized colloids in marginal solvents are ideal model systems for studying aggregation caused by pure attractions of moderate strength (~1–5 k_BT). Neutron scattering experiments are not only ideal to monitor the particle and suspension structure at different volume fractions, they also provide detailed insight into the crucial influence of temperature on the stabilizing polymer shell as the origin of the attractive interaction.

These experiments were performed using particles with a partially deuterated core that allowed us to use different contrasts for the core and the shell through systematic contrast variation (Zackrisson et al., 2005 & 2006). Contrast variation, through isotopic exchange of both core and solvent, then allows us to shift the focus from the overall, composite particle to the PEG layer, which we studied both in the dilute limit and as a function of particle concentration. Figure 3 provides an example of the enormous variations in the scattering curves that result from these different contrasts, also indicated as an inset in Figure 3B. These experiments clearly indicated that no detectable change in PEG layer properties occurs as a function of particle concentration, up to moderate concentrations. On diminishing the solvent quality, subtle changes in the PEG layer however became clearly visible that translate into attractions among particles. Using appropriate theoretical models, it was then possible to estimate the magnitude of these interactions and demonstrate that they vary smoothly with solvent quality such that the particles can be made to aggregate in a fully reversible fashion.

Experiments that shed light onto the particularly important case of strongly attracting particles at high volume fractions, i.e. in the upper right corner of Figure 2, are particularly challenging. While these suspensions typically are highly turbid and thus exclude normal light scattering experiments, their characteristic length scales are such that they are at the limit of standard SANS experiments, and their related dynamics are so slow that NSE experiments are out of question. Here we have thus designed a combined time-resolved SANS – light scattering experiment, where SANS was performed using a set-up with neutron lenses in order to enlarge the accessible q-range and the experimental resolution, and the light scattering experiments were performed using diffusing wave spectroscopy that provides access to short time dynamics on length scales similar to those accessed by SANS (Rojas et al., 2003; Vavrin et al., 2004; Vavrin, 2005). The experimental design that combines a typical SANS experiment and a DWS set-up is shown in Figure 4. Figure 4A schematically shows the combination of neutron lenses to enhance the low-q range, and a DWS set-up that

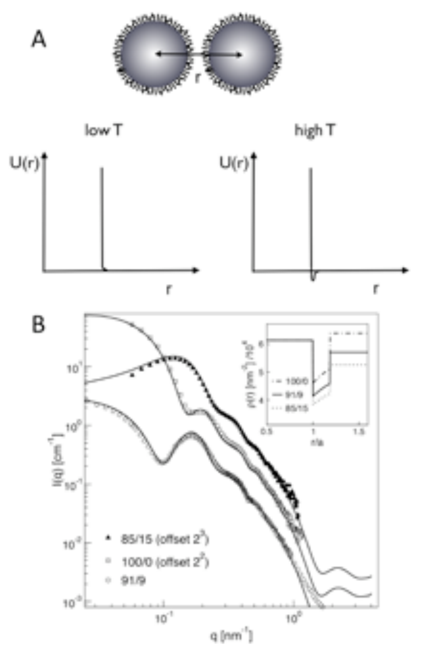

Figure 3: A) Schematic representation of the interaction potential between the particles under good and poor solvent conditions.
B) Scattering intensities as a function of scattering vector for core shell particles at three different contrasts as indicated in the inset. (Zackrisson et al., 2005 & 2006).

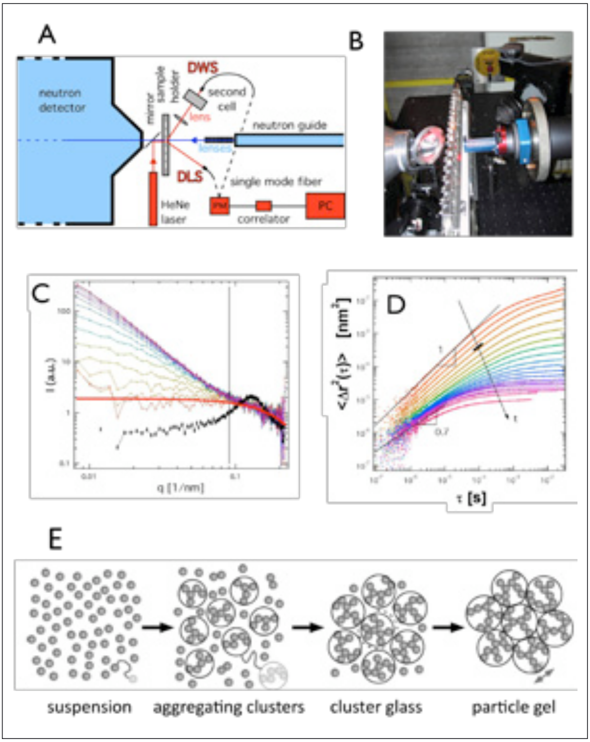

Figure 4:
A) Schematic view of the combined SANS and DWS experiment.
B) Picture of the actual set-up implemented at the SANS I Instrument at SINQ.
C) Time-evolution of the scattering intensity I(q) as a function of q from SANS for a destabilized colloidal suspension. Also shown is the intensity of the initial charge-stabilized suspension (black curve) and the form factor of the individual particles (red curve).
D) Mean square displacement of the particles from DWS as they aggregate and form a gel. The time increases in direction of the arrow; the short line indicates the point where the system starts to exhibit non-ergodic behavior.
E) Schematic gelation process that includes a cluster glass phase before a gel is finally formed. (Vavrin et al., 2004; Vavrin, 2005).

provides dynamic data on the time dependence of the average particle mean square displacement $\langle \; r^2(\;)\rangle$, while Figure 4B shows an actual picture of the set-up.

The resulting static and dynamic data obtained during a sol-gel process of a concentrated and fully destabilized colloidal suspension are shown in Figures 4 C and D. Figure 4C shows the evolution of the individual clusters with time, which can be compared to the structure factor of the initial charge-stabilized suspension and the scattering from the individual non-interacting particles. We clearly see an increase in the forward scattering due to the growing cluster size due to the irreversible aggregation of the destabilized particles, which slows down and eventually arrests as the system forms a gel. At the same time the particle dynamics continues to evolve as shown in Figure 4D, with a typical arrested subdiffusive motion of the particles as soon as the system arrests, where the maximum mean square displacement however continues to decrease while the gel stiffens due to continuing formation of bonds between the individual clusters that seems to follow a kind of percolation process.

A systematic investigation of the temporal evolution of the structure and the dynamics of the system as it undergoes a sol-gel transition has provided us with a qualitative picture as summarized in Figure 4E. Initially the stable colloidal suspension is destabilized for example through the addition of salt, and particles aggregate into growing clusters. Throughout this aggregation phase the clusters still undergo free diffusive Brownian motion. This changes when a glass like state is established where the clusters form cages that inhibit free motion of clusters outside their cages, and then the clusters interconnect and build a system-spanning and stress-bearing network, the gel. The investigations summarized in Figure 4 are a good example for the importance of conducting neutron scattering experiments together with complementary tools in order to cover the necessary length and time scales.

A COLLOID APPROACH TO DENSE PROTEIN SOLUTIONS AND MIXTURES

Colloid physicists make extensive and successful use of globular proteins as model colloids to gain a better understanding of various phenomena in colloid science. The reasons for the popularity of biocolloids or biopolymers, as proteins are often referred to in the colloid community, are manifold. It is basically a combination of outstanding qualities such as perfect monodispersity of single chain proteins, the possibility to tune their surface charge simply by pH, the occasional existence of a temperature dependent short-range attraction, and a size of a few nm ideal for investigations using various scattering techniques, to name only the most important ones. However, the profit from using protein model systems is everything but unidirectional. It is in fact quite the contrary, as the colloidal models that emerge from this interdisciplinary research provide answers to numerous questions of high biological, physiological and medical relevance.

Understanding interparticle interactions in protein solutions is of central importance to gain insight into the origin of protein condensation diseases such as Creutzfeldt Jakob, Alzheimer, Parkinson or cataract, the leading cause of blindness worldwide. In our work we thus also exploit the close analogy between colloids and proteins and apply concepts from colloid physics to proteins in order to investigate and understand protein interactions and the resulting solution structure in dense protein solutions and mixtures (Stradner et al., 2004; Cardinaux et al., 2007; Gibaud & Schurtenberger, 2009). Here we demonstrate the importance of this colloid approach on a class of proteins that is vital for the understanding of cataract.

Cataract, a gradual clouding of the eye lens due to increased scattering of visible light, is an example of a protein condensation disease where concepts from colloid science could already help rationalize various properties of the protein solution comprising the eye lens (Bloemendal et al., 2004). The eye lens of mammals is an almost transparent aqueous solution of highly concentrated lens-specific proteins, the so-called crystallins. There are three major classes of eye lens crystallins, called α, β, and γ in order of decreasing size. The relative proportions and overall concentrations of the crystallins vary with position inside a given lens, with the concentration increasing from about 200 mg/mL in the cortex to about 400 mg/mL in the nucleus. The main task of the eye lens is to provide a highly transparent

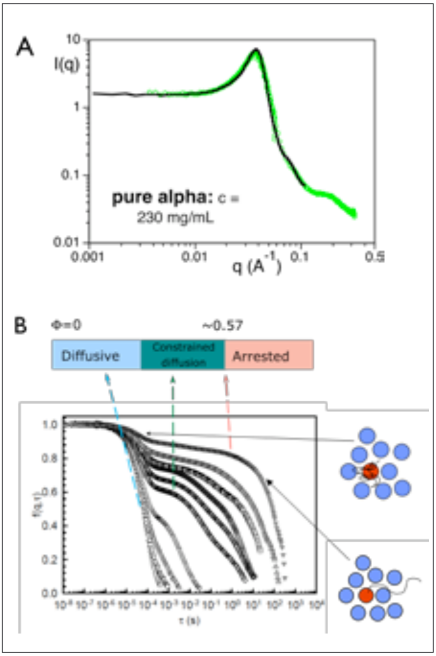

Figure 5: A) Comparison of experimental I(q) for α-crystallin solutions with the theoretical prediction for hard spheres.
B) DLS results for α-crystallin solutions with increasing concentration that exhibit the typical two step decay of a hard sphere colloid approaching the glass transition.

and highly refractive medium for proper focusing of the incoming light. A loss of transparency and thus visual acuity due to protein aggregation or phase separation leads to the formation of cataract, the leading cause of blindness worldwide.

Understanding the interactions between the crystallin proteins and their impact on lens transparency is therefore the first step towards a possible treatment of cataract. The behavior of the individual lens proteins has been shown to closely follow the predictions from simple colloid models. The α-crystallins are globular, polydisperse, multi-subunit proteins and their interactions can be described to a good approximation with a simple hard-sphere colloid model. This is illustrated in Figure 5, where results from a combined SANS and DLS study are shown. The SANS experiments demonstrate quantitative agreement between the predictions from hard sphere models and the measured q-dependent intensity. This is further supported by the DLS experiments, which show the existence of a glass transition again in quantitative agreement with hard sphere colloids and theory. The γ-crystallins on the other hand are much smaller and monomeric globular proteins. The discovery of the existence of a liquid-liquid phase separation that is metastable with respect to the solid-liquid phase boundary provided direct evidence for the existence of short-range attractions between γ-crystallins, and the use of the corresponding colloid model has led to a quantitative description of the solution properties arising mainly from scattering experiments and phase diagram studies (Schurtenberger et al., 1989).

While the individual crystallins have been well characterized, their mixtures are much less understood so far. Again a combination of SANS and Molecular Dynamics (MD) simulations has been key to obtaining a wealth of information on the interactions between the different species. Exploring the colloid-protein analogy we obtained evidence that weak attractions between unlike proteins are essential to guarantee and maintain lens transparency in an extremely sensitive and non-monotonic manner (Stradner et al., 2007; Dorsaz et al., 2009 & 2010). This novel finding of stabilization due to mutual attractions does not only represent an important step towards a better understanding of lens transparency, but also provides general guidelines for tuning the stability of colloid mixtures, a topic relevant for soft matter physics and industrial applications.

CONCLUSIONS

These few examples have shown our approach towards investigating soft matter, where we rely not only on neutron scattering, but combine it with a number of complementary techniques and often also with computer simulations. This has not only allowed us to gain considerable insight into equilibrium and non-equilibrium properties of colloidal suspensions, gels and glasses. Using the same approach, and based on the experimental and theoretical framework developed with colloidal model systems, we have been able to successfully draw analogies to complex systems from areas such as life, food and materials science. It is clear that the scientific progress made during these past 11 years of soft matter research in Fribourg would not have been possible without the availability of high-class experimental facilities such as SINQ, ILL or SLS. However, it is also important to point out that progress in this interdisciplinary area also crucially depends on a close collaboration between soft matter physicists, synthetic chemists capable of producing well defined model systems with tailored properties, and biologists, biochemists and materials scientists familiar with the even more complex systems that represent a worthwhile target for the research approach described in this article.

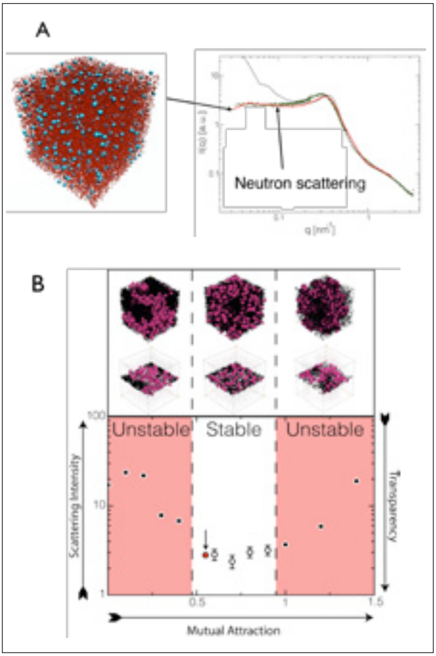

Figure 6: A) Comparison of experimental data and MD simulations for a weak mutual attraction between α- and γ-crystallins. Also shown is a comparison assuming pure hard sphere interactions between α- and γ-crystallins, and a snapshot from the simulations.
B) Stability diagram as obtained from MD simulations that shows the extent of the stable zone as a function of the strength of the mutual attraction between α- and γ-crystallins. (Stradner et al., 2007)

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Cation Dynamics in Ionic Liquids as Seen by Quasielastic Neutron Scattering

Jan Peter EMBS[1,2]

[1] Laboratory for Neutron Scattering, ETH Zurich & Paul Scherrer Institut, CH-5232 Villigen, Switzerland
[2] Physical Chemistry, Saarland University, D-66123 Saarbrücken, Germany

ABSTRACT

We report on quasielastic neutron scattering (QENS) investigations, performed to study the cation dynamics in the pyridinium based ionic liquid (IL) 1-N-butylpyridinium bis((trifluoromethyl)sulfonyl)imide. This IL allows for a detailed investigation of the dynamics of the cations only, due to its huge incoherent scattering cross section resulting from the cationic protons. The measured spectra can be decomposed into two Lorentzian lines, indicative for two distinct dynamical processes. The slower of these two processes is diffusive in nature while the faster one can be attributed to a localized motion. Using completely deuterated samples we can study the coherent dynamics which in turn affects the slow process as observed in the completely protonated sample.

INTRODUCTION

The class of ILs has attracted considerable research interest in the last few years and substantial progress has been achieved with respect to the knowledge on thermodynamic and transport characteristics of these compounds.

Concerning the structure of ILs, there is a huge number of research papers published on experimental as well as on theoretical investigations[1-14]. However the understanding of dynamics properties in ILs is still limited and many open questions remain to be answered. From recent simulations on ILs and also from experimental studies it became clear that the dynamics in these liquids is pronounced heterogeneous[5, 8, 12-13, 15-22].

Giraud[23] et al. studied the influence of cation and anion substitution on the ultrafast solvent dynamics of ILs by means of optical-Kerr-effect spectroscopy (OKE). The authors found three excitations in the wave number range between 30 and 100 cm^{-1}; these excitations have been attributed to out-of-plane librations of the Imidazolium ring of the cation. Later on, Xiao[24-26] et al. studied the anion effect in ILs with 1,3-pentylmethyl-imidazolium cations, using OKE method. The authors focus on the temperature dependence of the OKE spectra; the observed temperature dependence is attributed to the existence of inhomogeneities in the densities in these ILs; the densities are assumed to result from nanostructurally organized domains in the ILs, i.e. polar and non-polar regions. The existence of microphase segregation between polar and nonpolar domains in ILs was later on extensively studied by means of MD simulation techniques.

Voth and Wang[28] studied the influence of the length of the alkyl side-chain in Imidazolium based ILs on the aggregation of tail groups in these fluids. Increasing the number of carbon atoms in the side-chain shows that up to 3 carbons (C=3) no aggregation of tail groups takes place, while for $4 \leq C \leq 8$ an aggregation was observed. The case C=3 can be considered as a transition point dividing the liquids into those with or without tail aggregation on a microscopic scale. Lopes[29] and co-workers investigated the solvation of polar, nonpolar and association solutes in Imidazolium-based ILs; they found a site selective interaction between the solvent and the solute. The interaction of polar and nonpolar species was found to take place mainly with the cation.

Hu and Margulis[30] investigated by using MD simulation techniques the dynamics in the IL [1–butly–3–methylimidazolium]$^+$PF$_6^-$. Considering the mean-square-displacement (MSD) three distinct regions have been found: a ballistic region at short times, and intermediate "cage" region and a diffusive region a long times. Especially the behavior at intermediate times is of great interest since this plateau-like region is characteristic for supercooled liquids. By analyzing the van Hove correlation function it was found that most particles move slower than expected from normal Gaussian or Fickian diffusion; at the same time there exist subsets of particles that move much faster. Finally it is stated in this paper that the subgroups (both slow and fast) appear to be correlated in space. For supercooled liquids it is well known that the dynamics is slowed down before the transition to a glassy state; close to this transition, the dynamics in one region can be orders of magnitude faster than in a neighboring region only a few nm away; this is called spatially heterogeneous dynamics. This is in marked contrast to simple or ordinary liquids which are homogeneous.

The first paper on QENS investigations on 1-n-butyl-3-methylimidazolium hexaphosphate ([bmim][PF$_6$]) was published by Triolo and coworkers[31]. In the temperature range between 250 and 320 K two different relaxation processes have been observed. The faster of the two motions shows neither a Q- nor a T-dependence; this fast β-process was attributed to the motion of the molecules inside a cage. The slow α-process, on the other hand shows a non-Debye and non-Arrhenius behavior.

A recently published paper[33] deals with the investigation of the protic ionic liquid (PIL) N, N, N′, N′-tetramethylguanidinium bis(perfluoroethylsulfonyl)imide by means of QENS; this PIL could probably be used as an electrolyte in proton-conducting fuel cells. Above the melting temperature, i.e. in the liquid state, two processes have been observed. The first, slow, process, results from a true, unrestricted translational diffusion, while the second, fast, motion was described as spatially restricted translation diffusion.

Habasaki and Ngai[19] also used MD techniques to study the system $[EMIM]^+[NO_3]^-$. They also found signatures of heterogeneous dynamics in this IL and a strong coupling of the motion of both the anion and the cation. Finally Del Pópolo and Voth[35] discussed the heterogeneous dynamical behavior and argued that long living cages must exist, which are formed by neighboring ions. They observed a rattling of the ions inside the cage.

Despite all these efforts, a clear microscopic picture is still incomplete and thus highly demanding, since the dynamical properties of ILs are assumed to control in many ways their macroscopic properties.

SAMPLE PREPARATION

We used a two step synthesis[37] to get the IL 1-N-butylpyridinium bis((trifluoromethyl)sulfonyl)imide (see Fig.1).

The water content (< 4 ppm) was determined by means of Karl-Fischer titration.

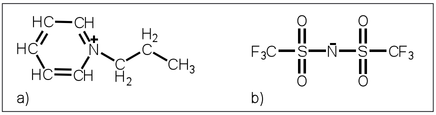

Figure 1: a) structure of the $[BuPy]^+$ cation and b) structure of the $[Tf_2N]^-$ anion.

Furthermore we used NMR-techniques to check purity and quality of partial deuteration. A completely protonated sample of [BuPy] $[Tf_2N]$ has an incoherent scattering cross section of about 1175 barn; the coherent scattering cross section is about 10% of this value. The main contribution to the incoherent scattering cross section comes from the hydrogen containing cation, while the contribution from the anion is negligible. For that reason QENS allows for a detailed investigation of the single-particle dynamics of the cations. The influence of the 10% coherent scattering contribution will be discussed later.

NEUTRON SCATTERING EXPERIMENTS

The method of quasielastic neutron scattering[38] (QENS) is suited to study stochastic, i.e. non-periodic dynamic processes[39] in condensed matter. In principle the method allows for an investigation of true (long-range) diffusion, localized processes (reorientations) and jump diffusive motions. The aim of QENS experiments is to extract diffusion coefficients, jump lengths and reorientation times. Incoherent QENS is very sensitive to samples containing hydrogen due to the large incoherent scattering cross section of this element.

The QENS experiments have been performed on the cold neutron time-of-flight spectrometer (tof) FOCUS[40] at the Swiss spallation source SINQ. For these experiments we used neutrons with an incident wavelength of $\lambda_i = 5.75$ Å. The energy resolution at this wavelength is (hwhm) $\Delta E \approx 22$ µeV. In this study we focus on temperatures, at which the IL is in the liquid state. All samples, including the 1 mm thick vanadium slab, were oriented at 135° with respect to the incoming neutron beam. The influence of the sample container was taken into account by subtracting the scattering intensities of an empty sample container. The measured intensities of the vanadium slab allow for an appropriate handling of the detector efficiency; furthermore these data have been used to determine the resolution of the spectrometer used. We employed measurement times of about 6 h for each temperature. Using the software package DAVE, the measured intensities were interpolated at constant Q and transformed from time-of-flight into the energy transfer domain; the Q range was reduced to values between 0.4 and 1.7 Å^{-1}. An example of a S(Q,E)-spectrum at Q = 1.1 Å^{-1} is shown in Fig. 2, together with the residuals as obtained by fitting the experimental data with an appropriate model (see section Data Analysis for further details).

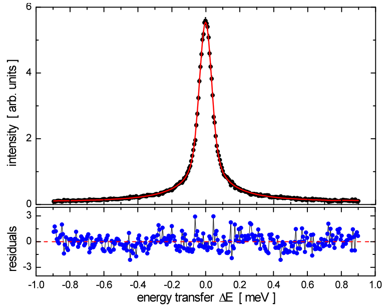

Figure 2: Upper panel: spectrum measured at 340 K and Q = 1.1Å^{-1} (symbols) together with the fit function (red solid line), described in the text. In the lower panel we show the residuals between the fit function and the measurement.

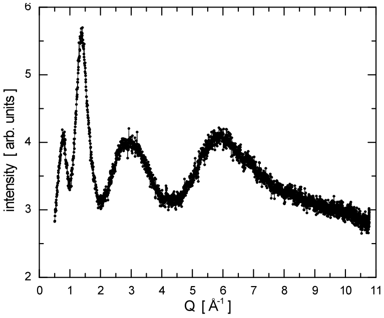

Figure 3: Intensity as function of Q as measured on a completely deuterated sample, $[BuPy]^+$ $[Tf_2N]^-$. This experiment was performed on the thermal neutron diffractometer HRPT at SINQ, using neutrons with $\lambda_i = 1.5$ Å.

We used a completely deuterated IL to study the structure in the liquid phase. The measurement was performed on the thermal diffractometer HRPT at SINQ. The main focus in this experiment was to get an overview about the occurrence of maxima in the measured intensity I(Q). As we will show later, the existence of maxima in the Q range, accessible in our QENS investigations, has marked influence on the dynamical properties. In Fig. 3 we plot the detected intensity as function of the modulus of the scattering wave vector. We see two rather narrow maxima below 2 Å^{-1}, followed by the expected broad oscillations at higher Q values.

DATA ANALYSIS

Model independent fits show that the measured quasielastic spectra can be very well described as a superposition of two Lorentzian curves, with very different linewidths. The standard procedure of dividing the QENS signal into an elastic (δ-like) part and into one or a sum of several Lorentzian (quasielastic part), was not applicable to our data.

Inspired by both, the fact that our measured spectra can be described in terms of two Lorentzian functions, as well as by the outcome of several MD simulations on similar systems, we decided to use a very general 2-state-model. This 2-state-model accounts for the existence of two different dynamical processes (states) and allows for transitions between these two states. This model was originally developed to describe the different states of water in solutions: one population of water molecules which is slow (bound to the ions, bond water) and a second population of water molecules which is described as bulk water. In the limiting case of slow exchange between the two states, the dynamic structure factor reads:

(1.)

$$S_{2sm}(Q,\omega)=\frac{1}{\pi}\left(n(Q)\frac{\Gamma_1(Q)}{\Gamma_1^2(Q)+\omega^2}+(1-n(Q))\frac{\Gamma_2(Q)}{\Gamma_2^2(Q)+\omega^2}\right)$$

The relative number of particles within the two states, $n_1(Q)$ and $n_2(Q)$, depend on the applied temperature and on Q. Since the relation $n_1 + n_2 = 1$ must hold for any value of Q, we introduced in Eq.1 the quantities n(Q) and 1-n(Q), respectively. The two linewidths (hwhm) $\Gamma_1(Q)$ and $\Gamma_2(Q)$ were considered to be free parameters, i.e. no specific assumptions about the Q-dependence were made.

The basic assumption is that in the IL (dynamically) different types of cations are present. The reason for this may be, for example, the fact that heterogeneities exist in the liquid. Furthermore we assume that the cations can perform transitions between the various types of dynamically different states. If the exchange between the states is slow, we can significantly simplify the dynamical structure factor S(Q,E).

The DAVE software package was used for data reduction and analysis. Data measured at constant scattering angles 2θ as function of the time-of-flight were transformed into Q-ω space. These data were binned into 14 groups of constant Q-values; the energy range was set to ±1 meV. During the data reduction process we took the contribution of the empty can into account. The data were normalized with respect to a standard vanadium cylinder.

The following form of the dynamical structure factor was used to fit the data:

(2.)

$$S(Q,E)=I(Q)\times S_{2sm}(Q,E)\otimes R(Q,E)+a+bE$$

The factor I(Q) contains an intensity factor and the usual Debye-Waller factor. With R(Q,E) we denote the resolution function, and represent a linear background. The convolution (denoted by the symbol ⊗ in Eq.2) is performed numerically using the PAN package as included in the DAVE software.

In Fig.2 we show a spectrum taken at 370K at Q = 1 $Å^{-1}$. The solid line in the upper panel of Fig. 2 represents a fit according to Eq. 2.

A closure inspection of the linewidth $\Gamma_2(Q)$ shows that these data can be very well described by a jump-diffusion model proposed by Singwi and Sjölander[41-42]. The linewidth in this model (which is in fact also a 2-state-model) is given by

(3.)

$$\Gamma(Q)=\frac{hDQ^2}{1+DQ^2\tau_0}$$

In **Eq.3**, D is the diffusion coefficient and with we denote the residence time, i.e. the time the particle spends at a position before performing the next jump event and thus reaching a new position.

RESULTS & DISCUSSIONS

In Fig.4 we show the linewidth (hwhm) $\Gamma_2(Q)$ as function of Q^2, for three different temperatures (300K, 340K and 380K). The data were fitted with Eq.3; in a first run we used all data points (dashed lines in Fig. 4), whereas in a second fit procedure (solid lines in Fig.4), we excluded those data points, which are close to the maximum of the static structure factor (see also Fig. 3).

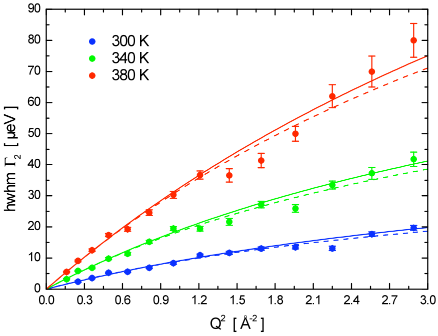

Figure 4: Linewidth Γ_2 (hwhm) as function of Q^2 for three different temperatures. The dashed lines are fits according to Eq.3, including all data points; the solid lines represent fits, in which the data points close to Q=1.3 Å^{-1} have been ignored (see text for further details).

From the two fitting approaches we extracted the diffusion coefficient D and the residence time , respectively. Both, the residence time as well as the diffusion coefficient are plotted as function of the inverse temperature in Fig.5; with filled symbols we represent those fit results, which were obtained by including all data points into the fitting procedure; open symbols represent fit results, which we got from excluding the data points in the neighborhood of the maximum of the structure factor from the fits.

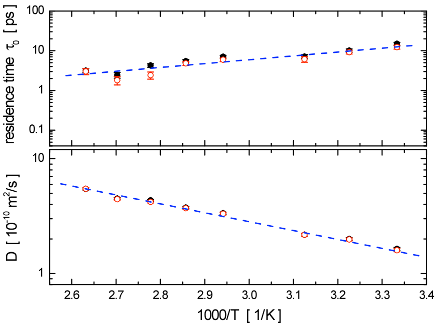

Figure 5: Upper panel: residence time T_0 as function of the inverse temperature. Lower panel: diffusion coefficient D as function the inverse temperature. Filled circles (black) represent results obtained by including all linewidth into the fitting procedure, whereas the open circles (red) are data, which have been obtained by ignoring those values of the linewidth Γ_2, which are close to the maximum of the static structure factor. The dashed lines are guides for the eyes.

The log-linear representations of data in Fig.4 imply Arrhenius-type activation processes[43]. We note here, that the diffusion coefficient D remains practically unaffected by the exclusion of certain data points from the fit, whereas the changes in the residence are more pronounced. These changes result from the fact that the data points, which were excluded from the fit process, are pretty far away from the low Q region, which in turn determine the diffusion coefficient. On the other hand, the residence time determines the large Q behavior, and thus modifying the data at large Q values, results in modified values for the residence times.

In order to study the role of the cationic alkyl chain and the pyridinium ring, we investigated completely deuterated samples in addition to the aforementioned completely protonated samples. In Fig.6 we compare the linewidth of the slow process as observed by fitting the data with the 2-state-model.

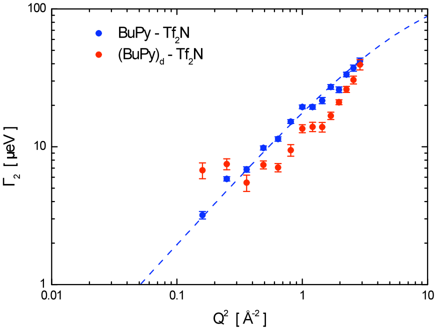

Figure 6: Comparison of fit results for the linewidth $\Gamma2$ of the slow process obtained from a completely deuterated and a completely protonated sample.
The slow process in the deuterated sample, as characterized by the linewidth $\Gamma2$ shows a clear slowing down at those Q-values which correspond to the location of maxima in S(Q).

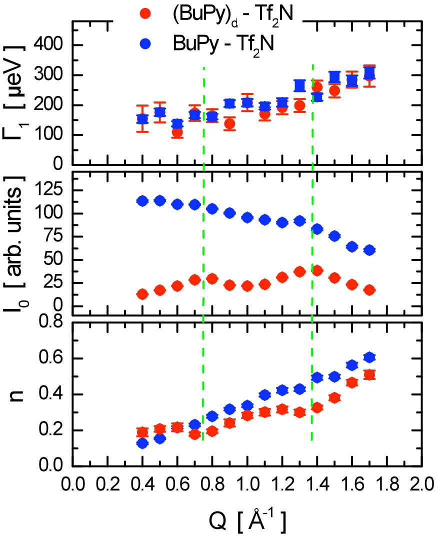

Figure 7: Comparison of fit results from a completely deuterated and a completely protonated sample. In upper panel we show the linewidth $\Gamma1$ of the fast process, in the middle panel we plot the intensity factor I(Q) and in the lower panel we show the fraction n of fast particles.

In Fig. 7, we compare the remaining fit parameters of the 2-state-model for the two samples used.

As can be seen from Fig. 7, the fraction of the fast particles/cations decreases at those Q values at which the static structure factor shows up with a maximum. This behavior is a clear signature for a slowing down of the dynamical process in the vicinity of maxima of S(Q). In the middle panel of Fig. 7 we plot the intensity factor as function of Q. In the case of the completely deuterated sample this factor is dominated by the behavior of S(Q), whereas in the completely protonated case this factor is affected by both, the static structure factor as well as by the Debye-Waller factor; the latter causes a intensity decrease for increasing Q values. The most interesting finding however is the fact, that the fast dynamical process remains unchanged by the static structure factor, as can be seen by inspection of the upper panel in Fig. 7. Furthermore we see a plateau-like behavior in $\Gamma_1(Q)$, which is indicative for a dynamical process inside a spatial confinement.

CONCLUSION & OUTLOOK

We used quasielastic neutron scattering to investigate the dynamical properties of the cation of the IL 1-N-butylpyridinium bis ((trifluoromethyl)sulfonyl)imide.

Quasielastic neutron scattering experiments, performed in the liquid state of the corresponding IL show up with (at least) two different dynamical processes, which take place on very different time scales. The first (slow) process is diffusive in nature; the linewidth which corresponds to this process can be very well described in terms of a jump diffusion process. By investigating a completely deuterated sample and comparing the linewidth of the slow process for both samples we can conclude that this process contains (in addition to incoherent scattering contribution) also coherent scattering components, thus being (at least partially) of collective nature.

The second (fast) process we observe, seems not to be affected by the structure, i.e. by the static structure factor S(Q). This experimental finding allows us to conclude that the fast process is a true single particle one, reflecting the single particle dynamical behavior on a short time scale. The fact that the linewidth of this process shows up with a plateau, may be interpreted as resulting from a process that takes place inside a confinement, which is formed by surrounding ions (both cations as well as anions).

The very general 2-state-model, that was used here to describe the QENS data, captures in a reasonable way the dynamical processes in the IL as observed with the instrumental resolution used. With increasing temperature the number of fast entities increases; this reflects the thermal activation of the processes; at the same time the number of slow particles decreases. The fact that we observe two fractions of cations (slow and faster ones) may be explained by the existence of dynamical heterogeneities in this IL; corresponding observations have been made by performing extended MD simulations on very similar ILs (see also the Introduction).

We will extend our investigations on ILs with increasing alkyl chain length (the basic cation and anion will remain unchanged) to study the influence of this length on the dynamical behavior that is observed with quasielastic neutron scattering as well as with fixed energy window scans to be performed on appropriate instruments. In a further step we will perform experiments with different instrumental resolutions and thus examine the influence of the observation times on the scattering data. Finally we will compare our results to results obtained with MD methods (classical MD as well as ab-initio MD simulations); due to the complexity of the ions the dynamical scenario is very complex and thus a combination of experiment and simulation is highly demanding.

ACKNOWLEDGEMENT

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Announcements

SGN/SSDN MEMBERS

Presently the SGN has 198 members. Online registration for new members of our society is available from the SGN website: http://sgn.web.psi.ch

SGN/SSDN ANNUAL MEMBER FEE

The SGN/SSDN members are kindly asked to pay their annual member fees. The fee is still **CHF 10.–** and can be paid either by bank transfer or in cash during your next visit at PSI. The bank account of the society is accessible for both Swiss national and international bank transfers. The coordinates are as follows:

Postfinance: 50-70723-6 (BIC: POFICHBE),
IBAN: CH39 0900 0000 5007 0723 6.

PSI FACILITY NEWS

PSI launched a **quarterly electronic newsletter** featuring recent news, events and scientific highlights of the three major PSI user facilities SLS, SINQ and SμS. The online version of the recent edition is available here: http://user.web.psi.ch/newsletter.

SINQ CALL FOR PROPOSALS

The next **deadline** for the submission of beam time requests for the Swiss spallation neutron source 'SINQ' (http://sinq.web.psi.ch) will be: **November 15, 2010.**

REGISTRATION OF PUBLICATIONS

Please remember to **register all publications either based on data taken at SINQ, SLS, SμS or having a PSI co-author** to the Digital User Office: https://duo.psi.ch. Please follow the link 'Publications' from your DUO main menu.

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Magnetic Phenomena

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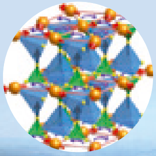

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Organizers

K. N. Clausen (chair);
R. Abela, G. Frei, S. Janssen,
M. Kenzelmann, E. Morenzoni,
C. Mudry, S. Müller, C. Quitmann,
J. F. van der Veen, A. Zheludev,
R. Bercher (secretary)

Scope

Magnetic phenomena are not only fascinating research topics, but also of key importance to a modern society. Magnetic phenomena and the understanding of these are basis for technologies with applications in information technology, energy conversion, diagnostics, sensors and actuators etc.

The school will introduce magnetism and strongly correlated electron systems and show how large scale facilities providing beams of photons, muons, and neutrons are used to study magnetic phenomena.

It is the second time that the PSI Summer School offers a twofold educational program with the traditional school in Zuoz followed by hands on training at the PSI Facilities in Villigen.

Invited speakers

External experts:

R. Allenspach, IBM Rüschlikon, CH; S. Blundell, Oxford University, UK; S. Bramwell, LCN, UK; S. Dudarev, UKAEA, UK; P. Gambardella, ICN, ES; P. Hedegård, University of Copenhagen, DK; H. von Löhneysen, KIT, DE; M. Kläui, Universität Konstanz, DE; S. Picozzi, INFM, IT; N. Shannon, University of Bristol, UK; M. Sigrist, ETHZ, CH; J. Valles, Brown University, US; H. Zabel, RUB, DE

PSI experts:

A. Fraile-Rodriguez, S. Gvasaliya, M. Kenzelmann, H. Luetkens, Z. Salman, T. Schmitt, M. Shi, J. Stahn, O. Zaharko, A. Zheludev (ETHZ/PSI)

Registration: http://school.web.psi.ch
Contact: renate.bercher@psi.ch (school secretary)

Deadlines:	**Early registration:**	**30 April, 2010**
	Regular registration:	**15 June, 2010**

Conferences and Workshops 2010/11

(an updated list with online links can be found here: http://sinq.web.psi.ch/sinq/links.html)

AUGUST

- HPSP14: 14th International Conference on High Pressure Semiconductor Physics
  August 1–4, 2010, Jilin, China
- M&M 2010 Microscopy and Microanalysis
  August 1–5, 2010, Portland, OR, USA
- PRICM – 07: 7th Pacific Rim International Conference on Advanced Materials and Processing
  August 1–6, 2010, Cairns, Australia
- ISSCG-14: International Summer School on Crystal Growth
  August 1–7, 2010, Dalian, China
- 59th Annual Denver X-ray Conference
  August 2–6, 2010, Denver, CO, USA
- X-ray Science in the 21st Century
  August 2–6, 2010, Santa Barbara, CA, USA
- CGOM9: 9th International Workshop on Crystal Growth of Organic Materials
  August 4–7, 2010, Singapore
- 2010 LANSCE Neutron School: Structural Materials
  August 5–13, 2010, Los Alamos, NM, USA
- 3rd K. H. Kuo Summer School of Electron Microscopy and Crystallography. International Workshop of 3D Molecular Imaging by Cryo-Electron Microscopy
  August 8–12, 2010, Beijing, China
- ICCG-16: International Conference on Crystal Growth
  August 8–13, 2010, Beijing, China
- 9th PSI Summer School on Condensed Matter Physics: Magnetic Phenomena
  August 7–15, 2010, Zuoz, Switzerland
- IMRC XIX: International Materials Research Congress
  August 15–19, 2010, Cancun, Mexico
- IMRC XIX: Symposium on Domain Engineering in Ferroic Systems
  August 15–19, 2010, Cancun, Mexico
- ANSTO Dynamics and Kinetics Neutron School 2010
  August 15–20, 2010, Sydney, Australia

- XIX International Materials Research Congress
  August 15–20, 2010, Cancun, Mexico

- XRM2010: 10th International Conference on X-ray Microscopy
  August 15–20, 2010, Argonne, IL, USA

- Gordon Research Conference on Solid State Studies in Ceramics. Fundamental Phenomena in Energy Applications
  August 15–20, 2010, New London, NH, USA

- XXth International Symposium on the Jahn-Teller Effect
  August 17–20, 2010, Fribourg, Switzerland

- IMA2010: Advances in Neutron Techniques in Earth and Environmental Sciences
  August 21–27, 2010, Budapest, Hungary

- ACS Fall 2010 National Meeting and Exposition
  August 22–26, 2010, Boston, MA, USA

- CUSO Villars Summer School in Materials: From Structure to Function in Nanomaterials
  August 22–26, 2010, Villars-sur-Ollon, Switzerland

- International Union of Materials Research Societies – International Conference on Electronic Materials 2010
  August 22–27, 2010, Seoul, Korea

- FEL 2010: 32nd International Free-Electron Laser Conference
  August 23–27, 2010, Malmo, Sweden

- JMC 12: Journees de la Matiere Condensee
  August 23–27, 2010, Troyes, France

- MSE2010: Materials Science and Engineering
  August 24–26, 2010, Darmstadt, Germany

- Combined 14th annual meeting of the Swedish Neutron Scattering Society and the final meeting of the Marie-Curie Training Network BIOCONTROL
  August 24–27, 2010, Lund, Sweden

- MECC2010: 5th Mid-European Clay Conference
  August 25–29, 2010, Budapest, Hungary

- MaThCryst Satellite Conference of ECM26
  August 27–29, 2010, Darmstadt, Germany

- EPDIC12: 12th European Powder Diffraction Conference
  August 27–30, 2010, Darmstadt, Germany

- ECM26: 26th European Crystallographic Meeting
  August 29 – September 2, 2010, Darmstadt, Germany

SEPTEMBER

- ECM Satellite Workshop: Methods of high-pressure single-crystal X-ray diffraction
  September 3–4, 2010, Darmstadt, Germany
- BACG 2010: British Association for Crystal Growth
  September 5–7, 2010, Manchester, UK
- Diamond 2010: 21st European Conference on Diamond, Diamond-Like Materials, Carbon Nanotubes, and Nitrides
  September 5–9, 2010, Budapest, Hungary
- BCA/CCP4 Summer School XV
  September 5–10, 2010, Oxford, UK
- Twelfth Annual YUCOMAT Conference
  September 6–10, 2010, Herceg Novi, Montenegro
- 14th JCNS Laboratory Course Neutron Scattering
  September 6–17, 2010, Jülich and München, Germany
- BIWIC 2010: 17th International Workshop on Industrial Crystallization
  September 8–10, 2010, Halle (Saale), Germany
- 5th Central European Conference: Chemistry towards Biology
  September 8–11, 2010, Primosten, Croatia
- 4th International SAXS/GISAXS Workshop
  September 9–11, 2010, Leoben, Austria
- 7th International Conference on Inorganic Materials
  September 12–14, 2010, Biarritz, France
- ICCBM13: 13th International Conference on the Crystallization of Biological Macromolecules
  September 12–16, 2010, Dublin, Ireland
- LINAC10: XXV Linear Accelerator Conference
  September 12–17, 2010, Tsukuba, Japan
- Metamaterials 2010: Fourth International Congress on Advanced Electromagnetic Materials in Microwaves and Optics
  September 13–16, 2010, Karlsruhe, Germany
- E-MRS 2010 Fall Meeting
  September 13–17, 2010, Warsaw, Poland
- BCA Industrial Group Autumn Meeting
  September 14–16, 2010, Almelo, The Netherlands
- ILL 2020 Vision: Future directions in neutron science
  September 15–17, 2010, Grenoble, France
- SGK/SSCr Annual Meeting 2010
  September 17, 2010, Geneva, Switzerland
- 88th Annual Meeting of the German Mineralogical Society: From Dust to Dust
  September 19–22, 2010, Münster, Germany

- Structure Under Extreme Conditions of Pressure and Temperature
  September 19–23, 2010, Gatlinburg, TN, USA

- IMC17: International Microscopy Congress

- IWN2010: International Workshop on Nitride Semiconductors
  September 19–24, 2010, Tampa, FL, USA

- 17th Bruker Users Group Meetings 2010
  September 20–22, 2010, Karlsruhe, Germany

- XTOP 2010: 10th Biennial Conference on High Resolution X-Ray Diffraction and Imaging
  September 20–23, 2010, Warwick, UK

- 10th International Symposium on Ferroic Domains and Micro- to Nanoscopic Structures
  September 20–24, 2010, Prague, Czech Republic

- SRI2010: 16th Pan-American Synchrotron Radiation Instrumentation Conference
  September 21–24, 2010, Argonne, IL, USA

- X School of Neutron Scattering Francesco Paolo Ricci: Electronvolt Neutron Spectroscopy of Materials: Microscopic Dynamics and Enabling Techniques
  September 25 – October 4, 2010, Rome, Italy

- International Workshop on Neutrons for Global Energy Solutions
  September 26–29, 2010, Bonn, Germany

- International School on Aperiodic Crystals
  September 26 – October 2, 2010, Carqueiranne, France

- Passion for Knowledge Workshops: Electrons, Photons, Interfaces, Soft Matter
  September 27 – October 1, 2010, San Sebastian, Spain

- HSC12: Synchrotron Radiation and Neutrons for Extreme Condition Studies
  September 27 – October 2, 2010, Grenoble, France

- 2010 Annual Meeting of the Mineralogical Society. Nuclear Waste Management: Research Challenges for the Future
  September 28–29, 2010, Cambridge, UK

- 6th International Workshop on Sample Environment at Neutron Scattering Facilities
  September 29 – October 1, 2010, Garching, Germany

OCTOBER

- XI RMS General Meeting on Modern Mineralogy: From Theory to Practice and the Fedorov Session 2010
  October 1–31, 2010, St Petersburg, Russia

- School on Imaging with Radiation
  October 1–2, 2010, Johannesburg, South Africa

- WCNR-9: 9th World Congress on Neutron Radiography
  October 3–8, 2010, Kwa-Maritane, ˆSouth Africa

- Barcelona BioMED Conference on Intrinsically Disordered Proteins in Biomedicine
  October 4–6, 2010, Barcelona, Spain

- CRISTECH 2010
  October 4–6, 2010, Autrans, France

- JCNS Workshop 2010 – Trends and Perspectives in Neutron Scattering: Magnetism and Correlated Electron Systems
  October 4–7, 2010, Bernried near Munich, Germany

- Nuclear Materials 2010
  October 4–7, 2010, Karlsruhe, Germany

- BioCrys 2010: Fundamentals of Modern Methods of Biocrystallography
  October 9–16, 2010, Oeiras, Prtugal

- NOBUGS 2010
  October 10–13, 2010, Gatlinburg, TN, USA

- 7th International Symposium on Superalloy 718 and Derivatives
  October 10–13, 2010, Pittsburgh, PA, USA

- IXS2010: 7th International Conference on Inelastic X-ray Scattering
  October 11–14, 2010, Grenoble, France

- X-ray Methods in Structural Biology
  October 11–26, 2010, Cold Spring Harbor, NY, USA

- Specimen Preparation for X-ray Fluorescence
  October 12–14, 2010, Newtown Square, PA, USA

- XI RMS General Meeting Modern mineralogy: from theory to practice and the Fedorov Session 2010
  October 12–15, 2010, Saint Petersburg, Russia

- Murnau Conference on Structural Biology: The Modern RNA World
  October 13–16, 2010, Murnau, Germany

- Third FRM II User Meeting
  October 15, 2010, Garching, Germany

- 3rd International Symposium on Transparent Conductive Materials
  October 17–21, 2010, Hersonissos, Crete, Greece

- Solidification and Crystal Growth Technology for Industrial Applications
  October 17–21, 2010, Houston, TX, USA

- Basic Rietveld Refinement and Indexing
  October 18–20, 2010, Newtown Square, PA, USA

- LCLS/SSRL Annual Users Conference and Workshops
  October 18–21, 2010, Menlo Park, CA, USA

- Materiaux 2010
  October 18–22, 2010, Nantes, France

- Advanced Rietveld Refinement and Indexing
  October 21–22, 2010, Newtown Square, PA, USA

- SENSE 2010: Superconductivity explored by Neutron Scattering Experiments
  October 22–23, 2010, Grenoble, France

- ICSAXS – 2010: International Conference on Applications of Small Angle X-Ray Scattering in the Field of Nanoscience and Nano Technology (no link available yet)
  October 23–24, 2010, India

- Neutron Reflectometry: the next generation and beyond
  October 25–26, 2010, Grenoble, France

- 68th Annual Pittsburgh Diffraction Conference
  October 27–29, 2010, Pittsburgh, PA, USA

- EMBO practical course on Solution Scattering from Biological Macromolecules
  October 25 – November 1, 2010, EMBL Hamburg, Germany

- Neutrons and Food
  October 31 – November 3, 2010, Sydney, Australia

- AsCA2010: Tenth Conference of the Asian Crystallographic Association
  October 31 – November 3, 2010, Busan, South Corea

NOVEMBER

- Polymorphism and Crystallization: Chemical Development Issues
  November 3–4, 2010, Clearwater Beach, FL, USA

- Advances in Protein Crystallography
  November 9–10, 2010, Florence, Italy

- SR in Earth, Space and Planetary Science - Exploiting the UK's newest facility
  November 10–11, 2010, Didcot, UK

- 3rd International Congress on Ceramics
  November 14–18, 2010, Osaka, Japan

- SARX 2010: XII Latin American Seminar of Analysis by X-ray Techniques
  November 15–19, 2010, Puebla, Mexico

- ENGE 2010: International Conference on Electronic Materials and Nanotechnology for Green Environment
  November 21–24, 2010, Jeju Island, Korea

- International Schools on Mathematical Crystallography
  November 22–27, 2010, Puebla, Mexico

- First North African Crystallographic Conference
  November 23–26, 2010, Casablanca, Morocco

- ICSOBA-2010: XVIII International Symposium
  November 25–27, 2010, Zhengzhou, China

- International School on Mathematical Crystallography
  November 29 – December 3, 2010, Montevideo, Uruguay

- MRS Fall Meeting
  November 29 – December 3, 2010, Boston, MA, USA

DECEMBER

- Annual Meeting of the Crystallographic Society of Japan
  December 3–5, 2010, Osaka, Japan

- XIPS 2010: 8th International Conference on X-ray Investigations of Polymer Structure
  December 8–10, 2010, Wroclaw, Poland

- CMMP10: Condensed Matter and Materials Physics
  December 14–16, 2010, Coventry, UK

- Pacifichem 2010
  December 15–20, 2010, Honolulu, HI, USA

CONFERENCES AND WORKSHOPS 2011

JANUARY

- International School on 'New developments in the Field of Synchrotron Radiation'
  January 17–25, 2011, Campinas, Brazil

- 5th International Symposium Hydrogen and Energy
  January 23–28, 2011, Stoos, Switzerland

JULY

- 5th European Conference on Neutron Scattering
  July 17–21, 2011, Prague, Czech Republic

AUGUST

- IUCr-2011: 22nd General Assembly and Congress of IUCr
  August 22–29, 2011, Madrid, Spain

SEPTEMBER

- JUM@P 11: Second Joint Users Meeting at PSI
  September 15–16, 2011, Villigen, Switzerland

Swiss Neutron Scattering Society
Sekretariat SGN/SSDN
Paul Scherrer Institut
WLGA/018
5232 Villigen PSI, Switzerland