SWEDISH NEUTRON SCATTERING SOCIETY

SNSS Annual Meeting

30-31 May, 2016
Lund, Sweden

THE NOBEL COMMITTEE
FOR PHYSICS
THE ROYAL SWEDISH ACADEMY OF SCIENCES

Vetenskapsrådet

This year's annual meeting of the Swedish Neutron Scattering Society, SNSS was held in Lund on 30th - 31st May.

The Swedish Neutron Scattering Society (http://snss.se) is a voluntary, non-profit organization of scientists working with neutron scattering and with the aim to promote and enlarge the community in particular in new areas of science. The ongoing construction of two major research facilities in Lund European Spallation Source (ESS) and the Max IV synchrotron are both central for advancing several scientific fields and also open up new opportunities for interdisciplinary collaboration.

Keynote speakers:

- Dr. Elizabeth Blackburn, Birmingham University
- Assoc. Prof. Stephen Hall, Lund University
- Prof. Matt Helgeson, UC Santa Barbara
- Prof. John White, The Australian National University

Organising Committee:
Andrew Jackson (European Spallation Source & Lund University)
Tommy Nylander (Lund University)
Zsuzsa Helyes (European Spallation Source)

Programme

Monday, 30 May 2016

12:00 Registration and Lunch

12:45 Welcome

13:00 VR Neutron Scattering Strategy - Presentation and Discussion
The Swedish Research Council, Vetenskapsrådet, has recently published its strategy for Swedish participation in the construction and hosting of the European Spallation Source [1].

[1] "Europeiska spallationskällan – ett världsledande verktyg för forskning, utbildning och innovation: Vetenskapsrådets förslag till strategi för svensk medverkan i och värdskap för ESS" http://www.vr.se

Leif Eriksson and Camilla Jakobsson from VR will present the strategy and take questions.

13:30 Discussion
Prof. Yvonne Andersson from Uppsala University will chair the session and moderate the discussion.

14:20 Instrumentation and Methods

14:20 '*Överlåtaren' a fast way to transfer and orthogonalize 2D offspecular reflectivity data* - Franz Adlmann (Uppsala Universitet)

14:40 *In-Situ Polarised Neutron Reflectometry During Thin Film Growth* - Wolfgang Kreuzpaintner (Technische Universität München)

15:00 Coffee Break

15:20 Hard Matter

15:20 Keynote: *Exploring large-scale magnetic structures - magnetic vortices and domains* – Elizabeth Blackburn (University of Birmingham, UK)

16:00 *Neutron scattering and spin ice* - Patrik Henelius (Theoretical Physics, KTH)

16:15 *A neutron scattering study of the hydride-ion dynamics in the novel perovskite oxyhydrides BaTiO3-xHx (x = 0.14 and 0.4)* - Carin Österberg (Department of Physics, Chalmers University of Technology, Sweden)

16:30 *Magnetostructural transition in Fe5SiB2 observed with neutron diffraction and the effect of P- substitutions* - Johan Cedervall (Uppsala University)

16:45 *Emergent magnetic order and topologically complex structures* - Pascale Deen (European Spallation Source ESS AB)

17:00 SNSS General Meeting

17:30 Community Interactions

17:30 *Support Laboratories in connection to ESS/MAX IV* - Lars Tilly (Innovation Skåne/Materials Business Center) Edvard Hall (Innovation Skåne/Materials Business Center)

17:45 *BrightnESS* - Ute Gunsenheimer (ESS - European Spallation Source ERIC)

18:00 Posters & Mingle

19:00 Dinner (until 22:00)

Tuesday, 31 May 2016

08:00 Coffee

08:30 Soft Matter

08:30 Keynote: *Toward "Damascus colloids": developing thermal processing strategies for colloidal gels* - Matthew Helgeson (UCSB)

09:10 *Deep Eutectic Solvents as media to promote surfactant self-assembly* - Adrian Sanchez-Fernandez (University of Bath)

09:25 *Using SANS to Investigate Soft Responsive Particles in Electric Fields* - Sofi Nöjd (Physical Chemistry, Lund University)

09:40 *Topological interactions in polymers under shear* - Maximilian Wolff (Uppsala University)

10:00 Coffee Break

10:20 Soft Matter

10:20 Keynote: *Probing Interactions Between Food Components* - John White (Australian National University)

11:00 *Molecular Structure of Trehalose-Water Solutions as Studied by Neutron Diffraction and EPSR Modelling* - Christoffer Olsson (Chalmers University of Technology)

11:15 *Manifestation of patchiness in small-angle scattering of proteins - it takes two to tango* - Malin Zackrisson Oskolkova (Assoc. Prof., Division of Physical Chemistry, Lund University)

11:30 Keynote: *Neutron imaging of mechanical and hydromechanical processes in rocks* - Stephen Hall (ESS / Lund University)

12:00 ESS Construction Site visit

13:00 Lunch at ESS

14:00 MAX IV Lab visit (until 15:00)

Abstracts

1 Instrumentation and Methods

1.1 'Överlåtaren' a fast way to transfer and orthogonalize 2D offspecular reflectivity data - Franz Adlmann (Uppsala University)

Neutron reflectivity techniques offer several unique opportunities in materials research. However the possibility to fully take advantage of the data being taken depends entirely on the software available for analysis and visualization.

This limitation becomes obvious in terms of accessing off-specular data in momentum transfer space [1]. This is a specific capability, which has been proven to be needed for the analysis of hierarchical structures [2] as often found in soft matter [3] and 3D magnetic structures [4].

We present a new program package, that conducts generic 2D transformations to an orthogonal grid. It is specifically set for transferring instrument data into momentum transfer space. The method is designed and optimized for repeatable operations as they occur as standardized instrument settings being common on large scale facilities

In this contribution, we prove the operational capabilities of our package by showing artificial and real data from instruments at ORNL and ILL.

Further the limitations and an outlook for future capabilities and applications, such as coherent reflectivity [5] and true background reduction, will be presented.

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[3] M. Wolff, A. Magerl et al. , Eur, Ohys. J. E (2005). 16, 141-145
[4] E. Kentzinger, et.al. , Physica B (2003). 335, 82-88
[5] W. A. Hamilton, et al., Journal of Neutron Research (1994). 2, 1-19

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1.2 In-Situ Polarised Neutron Reflectometry During Thin Film Growth - Wolfgang Kreuzpaintner (Technische Universität München)

Thin magnetic layers and heterostructures are the basic building blocks of a large number of magneto-electronic devices. While the structural characterisation of thin films during growth by various techniques is common practice (as e.g. commonly done by RHEED/LEED, STM or synchrotron radiation), the in-situ measurement of the magnetic properties of films using (polarised) neutron reflectometry is a challenging task. Within a collaboration of TU München, University Augsburg and MPI Stuttgart, we operate a mobile sputtering facility for the growth and in-situ monitoring of magnetic multilayers, which can be installed at suitable neutron beamlines. In our contribution, the setup and first proof of principle polarised in-situ neutron reflectivity measurements on in-situ grown Fe/Cr carried out at the ToF reflectometer REFSANS at the FRM II neutron source and at the AMOR beamline at PSI will be presented. At the latter, use of the Selene neutron optical concept allows very fast polarised neutron reflectivity measurements to be performed within only 15min per spin direction.

2 Hard Matter

2.1 **Keynote: Exploring large-scale magnetic structures - magnetic vortices and domains -** Elizabeth Blackburn (University of Birmingham)

Often, when thinking of magnetic structures, the textbook picture is of magnetic moments on individual atoms, engaged in collective action to form ordered or partially ordered states. Neutron scattering has proved essential as a direct probe of these magnetic structures. In this experimental paradigm, the existence of meso- or microscopic magnetic structures is, perhaps, an irritation or potential source of error. In many cases, however, these larger structures provide a clear view of the underlying state of matter, or drive the observable magnetic phenomenology. In this talk, I will consider two areas where these larger structures are crucial: (i) magnetic vortices as a tool for probing the superconducting state, and (ii) magnetic domains and their role in driving magnetic transitions in materials.

2.2 **Neutron scattering and spin ice -** Patrik Henelius (Theoretical Physics, KTH)

The spin-ice family of materials is one of the foremost realizations of a frustrated magnetic system displaying a macroscopic ground state degeneracy down to sub-Kelvin temperatures. Neutron scattering is a sensitive probe of the magnetic correlations in these materials, and one of the primary methods used to constrain the free parameters of the Hamiltonian. We will give specific examples of the uses of neutron scattering techniques applied to frustrated magnets. In particular we discuss recent efforts to elucidate the possibility of an ordered ground state in the spin-ice material Dy2Ti2O7.

2.3 A neutron scattering study of the hydride-ion dynamics in the novel perovskite oxyhydrides BaTiO3-xHx (x = 0.14 and 0.4) -

Carin Österberg (Department of Physics, Chalmers University of Technology, Sweden)

Proton conducting perovskite type oxides, such as BaTi1-xYxO3Hx, for which the protons are covalently bound to oxygens, are currently accumulating considerable attention. The proton conduction mechanism may be divided into two principal processes, hydrogen-bond mediated proton transfers (jumps) between neighbouring oxygen ions, and -OH reorientational motion between such transfers[1]. However, the local chemistry and structure, symmetry reduction, hydrogen-bonding interactions and proton-defect interactions etc., complicate the description about proton dynamics that is still not fully understood for even the simplest systems. A novel possibility to advance the understanding of hydrogen dynamics in perovskite materials is given by the recently discovered perovskite oxyhydrides ATiO3-xHx (A = Ba, Sr, Ca, x < 0.6)[2]. The hydrogens in oxyhydrides is of hydridic nature (H-) and take the place of oxygen vacancies rather than being covalently bound to oxygens. In contrast with most other oxyhydrides, ATiO3-xHx are stable in air up to ca. 400 C, above which hydrogen is released. This observation leads to the conclusion that the hydride species in ATiO3-xHx have to be mobile. This finding is highly exciting because it implies that the perovskite structural framework can accommodate both, cation (proton) and anion (hydride) conduction.

Here, we report on investigations of both the local structure and dynamical behavior of the oxyhydride BaTiO3-xHx (x = 0.14 and 0.4), by means of inelastic (INS) and quasielastic neutron scattering (QENS). The INS results show two strong bands at 912 and 1027 cm-1 which are assigned to the Ti-H vibrations[3] and confirm the absence of a O-H band at approximately 3500 cm-1. Hence the results verify that the hydride-ions are located on vacant oxygen sites of the perovskite lattice. Subsequent measurements of the mean-square displacement of BaTiO3-xHx (x = 0.4) show a marked increase in the temperature range ca. 300-400 K, which indicates that there is a displacement reflecting the onset of diffusional H motion. Measurements of quasielastic spectra for T = 275-500 K indicate the presence of hydride-ion dynamics characterized by a relaxation time of the order of one nanosecond.

[1] M. Karlsson, Dalton Trans. 42 (2015) 317.
[2] Y. Kobayashi et al., Nature Mater. 11 (2012) 507.
[3] Y. Iwzaki et al., J. Appl. Phys. 108 (2010) 083705.

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2.4 **Magnetostructural transition in Fe5SiB2 observed with neutron diffraction and the effect of P- substitutions -** Johan Cedervall (Uppsala University)

Permanent magnets are highly used in energy applications, both for harvesting in e.g windmills and for usage in electric vehicles. To reduce the price tag for the manufactured magnets expensive elements like Nd, Gd and other rare earth elements should be avoided. Therefore other types of rare earth free permanent magnets are currently under heavy research. However, rare earth elements have a strong spin-orbit coupling with transition metals which gives the structures high magnetocrystalline anisotropy energy, a structural property that can give the material good magnetic properties. To overcome this without rare earth elements, uniaxial structures should be used, like tetragonal τ-phase MnAl or FeNi. Another material with a uniaxial tetragonal structure that is rich in Fe-atoms is the compound Fe5SiB2. Fe5SiB2 crystallises in the space group I4/mcm and have two crystallographically different iron sites that orders ferromagnetically at 760 K, magnetic measurements have also indicated that a magnetic reorientation takes place at 172 K. Therefore investigations with neutron powder diffraction were performed on the D1B beamline at ILL (Grenoble, France) and the results revealed that orientations of the magnetic moments at high temperatures are along the crystallographic c-axis. Below the magnetic transition the orientation changed to the a-axis which confirms the proposed spin-flip transition. The magnetic properties can be tuned by substitutions and therefore the effects of P in the Si-sites were studied since the magnetic anisotropy are supposed to increase with P-content according to first principle calculations. However, the spin-flip is inhibited by P-substitutions.

2.5 Emergent magnetic order and topologically complex structures - Pascale Deen (European Spallation Source ESS AB)

The search for new states of matter is a fundamental theme of condensed matter science. Frustrated magnetic materials are promising candidates for new states because lattice geometry suppresses conventional magnetic dipole order. Frustration thus drives novel emergent states. Classical spins on the 3D triangular hyperkagome lattice have long been considered ideal for novel states yet have provided few examples. Gd3Ga5O12 is the canonical frustrated magnet since the compound does not order via the pervasive “order by disorder” mechanism down to the lowest temperatures probed, 25 mK [1 and ref. therein]. Short-range correlations, determined via neutron diffraction, have long been assumed to originate from near neighbour short-range interactions [1]. However in recent work an emergent spin state of decagon looped structures at the lowest temperatures has been uncovered [2,3]. These emergent decagon spin loops remain dominant when attempting to polarise the spin structure by a large applied magnetic field [4]. Neutron inelastic scattering shows a dominant contribution at large momentum transfers from a band of almost dispersionless excitations that correspond to the spin waves localized on ten site rings, expected on the basis of nearest neighbor exchange interaction [4]. These result illustrate the richness and diversity that arise from frustrated exchange on the three-dimensional hyperkagome lattice.

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[4] N. d’Ambrumenil, O.!A. Petrenko, H. Mutka, and P.!P. Deen, Phys. Rev. Lett. 114, 227203 (2015)

3 Community Interactions

3.1 **Support Laboratories in connection to ESS/MAX IV -** Lars Tilly (Innovation Skåne/Materials Business Center) Edvard Hall (Innovation Skåne/Materials Business Center)

Materials Business Center is conducting a pre-study on the supporting laboratory resources to be built in connection to ESS and MAX IV in Lund to facilitate for external usage of the research facilities by users with limited experience in conducting these types of experiments.

They carry out this study on behalf of Lund university/MAXIV, ESS, Region Skåne and Science Village Scandinavia and are reaching out to academia and industry, both in Sweden and internationally, to get an understanding of their needs in terms of designing experiments, preparing the samples and interpreting the results. During this session, the interim conclusions will be presented and the presenters will seek input from the audience.

In particular, the pre-study addresses the following questions:
1. Is there need within industry and academia to have supplementary scientific infrastructure around ESS and MAX IV, for the design and preparation of experiments and subsequent result analysis?
2. If there is such a need, what kind of lab equipment should be included?
3. What laboratory resources are needed? Can they be collected in a small number of groups of laboratories (as in Grenoble with regard to structural Biochemistry).
4. How can a general structure of laboratories be put together in order to attract relevant companies and academic institutions to be part of an establishment process?
5. What should the process of detailing the content and create a business/financial plan look like?
6. What parties are the most relevant and engaged in moving such a process forward, as a core group of the implementation phase?
7. What can be learnt from the establishment processes in other European examples such as from ISIS and Diamond in Oxford, around Helmholtz Zentrum in Berlin and ILL and ESRF in Grenoble?

3.2 ***BrightnESS*** **-** Ute Gunsenheimer (ESS - European Spallation Source ERIC)

The European Union has identified ESS as one of a handful of strategic research infrastructures necessary to keep Europe at the forefront of scientific knowledge.

Acknowledging the strategic relevance of ESS, the European Union financially supports its successful construction through BrightnESS, a three-year programme (September 2015 - August 2018) implemented by 18 European partners.

Fully integrated with the ESS project, BrightnESS:

- Facilitates the transition of ESS from its initial phase to its new status as an ERIC;
- Supports the development, testing and optimization of state-of-the-art technology in neutron detectors;
- Develops real-time management of the data taken on ESS instruments;
- Strengthens the In-Kind Contribution process;
- Engages with existing and potential stakeholders (scientific, industrial and academic partners, government representatives, students and educators, and society at large);
- Fosters a collaborative spirit through active knowledge-sharing.

BrightnESS is funded by the European Union Framework Programme for Research and Innovation, Horizon 2020, under grant agreement 676548. Budget: 19, 941 954 M €

4 Soft Matter

4.1 Toward "Damascus colloids": developing thermal processing strategies for colloidal gels - Matthew Helgeson (UCSB)

The ability to control phase separation in molecular media (including metals, ceramics, minerals and polymers) is a conserved motif for designing mesostructured materials that spans antiquity, modern technology and the natural world. In particular, sophisticated quenching and annealing strategies to create bicontinuous or hierarchical morphology have allowed for the creation of materials with significantly enhanced mechanical and transport properties.

However, developing such processing strategies for colloids poses significant challenges, including relatively slow dynamics and a lack of scalable material systems in which colloidal interactions can be actively tuned and quenched. To overcome these challenges, we have developed a colloidal system based on stimuli-responsive, self-assembling nanoemulsions that allows for fine control over their interdroplet attractions and resulting colloidal phase separation. We have used these nanoemulsions to understand how long-range, thermoreversible colloidal attractions can be used to assemble droplets into arrested bicontinuous liquid template structures with controlled length scales of porosity.

Here, I will show how neutron scattering measurements, and accompanying statistical mechanical modeling, have been critical to understanding the colloidal interactions and assembly mechanisms that underlie these new quenchable colloidal gels. Furthermore, we find that controlling arrested phase separation in these gels results in significantly enhanced mechanical toughness.

Finally, I will show how we use advanced "rheo-SANS" methods, which combine rheological measurements with in situ neutron scattering, to understand the mesoscale processes that give rise to superior mechanical properties.

4.2 **Deep Eutectic Solvents as media to promote surfactant self-assembly** - Adrian Sanchez-Fernandez (University of Bath)

Deep eutectic solvents (DES) have attracted a wide interest as alternatives to traditional solvents due to their green character and potential designability of the solvent properties. DES show a melting point near or below room temperature with a relatively low vapour pressure, high thermal and chemical stability and wider liquid temperature range than molecular solvents. Furthermore they are composed of non-toxic, cheap precursors.[1]

Our first study has revealed that interactions between solvent and surfactant headgroup play an important role in the micellization process. We therefore aim to establish how the characteristics of the solvent influence the self-assembly of surfactants. Here we will present our recent studies in the aggregation of an anionic surfactant, sodium dodecylsulfate (SDS), in the widely studied choline chloride:urea deep eutectic solvent [2]. Scattering techniques were used to determine the characteristics of the aggregates. Small-angle scattering has shown the formation of elongated aggregates, different to the behaviour of SDS in other polar solvents which forms globular-like micelles. Furthermore a rather uncommon rod-to-globular shape transition was found with increasing the concentration of surfactant. We will present details of surfactant self-assembly and changes in the system with surfactant concentration, temperature and water content.

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4.3 **Using SANS to investigate soft responsive particles in electric fields -** Sofi Nöjd (Physical Chemistry, Lund University)

Soft and deformable ionic microgels such as poly(N-isopropyl-acrylamide) co-acrylic acid (PNIPAM-co-AA) microgels have shown to be well suited as model systems to study the phase behaviour found for particles interacting via a soft isotropic potential. Additionally, subjecting these particles to an alternating electric field induces a dipolar contribution to the interaction potential, which strongly depends on the amplitude and frequency of the applied field. This additional, tunable and directional attraction allows us to explore and deepen our understanding of systems interacting via an even more complex anisotropic potential.

In the dilute regime, previous studies using confocal microscopy have shown that the system undergoes a fluid to string-fluid transition with increasing field strength [1]. At high densities, we see that a face-centred cubic (FCC) crystal diffusively transforms into a body-centred tetragonal (BCT) crystal through a nucleation and growth mechanism. Surprisingly, when turning off the field the system does not relax back to the stable FCC phase, but transforms into a long-lived metastable body-centred orthorhombic (BCO) phase through a non-diffusive martensitic transition [2]. Currently the reason for this path-dependent sequence of crystal-crystal transitions is not clear, and we need more information about the effective interaction potential between the particles. Moreo-ver, given the softness of the microgels, the particles can also shrink, interpenetrate and deform upon string formation, and thus the resulting potential will strongly depend upon the actual particle size and shape as a function of field strength and particle concentra-tion. This requires high spatial resolution, and we thus use small-angle neutron scatter-ing experiments under so-called zero average contrast conditions in order to extract the single particle structure as a function of an increased field strength. We present results obtained using a custom-made sample environment that allows us to study the size and shape of individual particles in-situ while they undergo field-induced transitions to string fluids or ordered colloidal crystals.

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4.4 **Topological interactions in polymers under shear -** Maximilian Wolff (Uppsala University)

Polymers show very interesting flow properties with increasing deformation related to changes of the storage and loss moduli. Ideally, these macroscopically observable changes can be linked to the microscopic structure and dynamics. Getting a direct handle on the microscopic quantities is challenging since scattering experiments on in-situ sheared polymers are difficult. We have constructed a custom made shear device to allow in-situ scattering experiments on high molecular mass polymers at Weissenberg numbers larger than one. We developed a neutron spin echo based approach that for the first time allows to in situ monitor nano-scale dynamics in flowing media and report evidence for a transition in the topological interactions in high molecular mass polydimethylsiloxane. This transition is only traceable in the single chain dynamics but not linked to structural rearrangements.

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4.5 Probing Interactions Between Food Components - John White (Australian National University)

A model for foods is to consider them in terms of colloidal composites. Great progress has been made in understanding colloidal systems and their interfaces using x-ray and neutron scattering but especially with contrast variation of one or both of the components. For colloids, the interactions between the components are relatively weak electrostatic and van der Waals forces. Even the major components of some foods, the proteins, are relatively fragile to heat, interfacial stresses and pressure as well as the pH of the system. All of these stresses appear in foodstuff processing as well as compositional variability.

Milk is a substance of relatively constant composition and so will be taken as one of the examples in the lecture. The accessibility of scattering methods to understanding the weak interactions between caseins and inorganic phosphate will be discussed.

A challenge – already resolved for simple colloidal systems – is the use of deuterium substitution for neutron scattering contrast in foods. This is well developed for some proteins and membrane structures but only now being achieved for the caseins in milk. Most proteins are robust to deuteration but others not – this may be a problem to solve.

4.6 Molecular Structure of Trehalose-Water Solutions as Studied by Neutron Diffraction and EPSR Modelling - Christoffer Olsson (Chalmers University of Technology)

The di-saccharide trehalose has been the focus of a lot of research during the past two decades due to its superior ability to stabilize biological macromolecules in extreme conditions. A more fundamental understanding of the molecular properties of trehalose in solutions may lead to improved preservation techniques, such as improved food and medication storage, or successful cryopreservation of human organs for transplantations.

We are currently studying the structural properties of trehalose-water solutions using neutron diffraction, with six different isotope compositions, and Empirical Potential Structure Refinement (EPSR) modelling. Using this approach, we should be able to answer important questions regarding how trehalose interact with water and thereby perturb the hydrogen bonded network of water. We should also be able to determine the intramolecular structure of individual trehalose molecules in the solution, and whether the trehalose molecules form clusters or are more homogeneously dispersed in the water.

Preliminary results indicate that the water structure is significantly perturbed by the presence of trehalose, and that water form plenty of hydrogen bonds with trehalose primarily via the hydroxyl groups of trehalose, and particularly with the hydroxyl groups on the methyl groups. Furthermore, there is no indication of any significant clustering of trehalose.

The improved understanding of the structural properties of this sugar solution will also be beneficial for our future studies of proteins in the same solution, where we aim to understand the extraordinary stabilizing effect of trehalose on proteins.

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4.7 **Manifestation of patchiness in small-angle scattering of proteins - it takes two to tango -** Malin Zackrisson Oskolkova (Assoc. Prof., Division of Physical Chemistry, Lund University)

We present a robust framework for pinpointing patchy intermolecular interactions from scattering data. Our analysis is based on a SAXS/SLS study of the milk protein lactoferrin which forms highly stereo-specific dimers, resulting in a non-monotonic dependence of the second virial coefficient on electrolyte concentration. The results are interpreted using an integral equation theory that accounts for isotropic, electrostatic repulsion and a directional patch that allows for dimers, but precludes trimer formation. This model captures the complete transition pathway from monomers in the dilute limit, to monomer-dimer systems at somewhat higher protein concentrations.

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4.8 **Neutron imaging of mechanical and hydromechanical processes in rocks -** Stephen Hall (ESS / Lund University)

Understanding the mechanisms of deformation and failure in rocks and their implications for fluid-flow and -storage are key to a number of important industrial/environmental applications, including geologic CO_2 sequestration and hydrocarbon production. The common method to analyse the deformation behaviour of rocks is triaxial compression testing where an axial load is applied to a sample under some confining pressure, which aims to simulate subsurface conditions. In such tests, stress and strain are measured at the boundaries of the sample and fluid flow can be measured by monitoring flow rates or fluid pressures at the ends of the test specimen. The standard interpretation of such data requires assumptions of homogeneity of the samples and the properties being measured/inferred. Unfortunately, this assumption is very rarely valid, as rocks are generally heterogeneous and failure occurs through some localised phenomena, such as strain localisation or fracture, which implies heterogeneity of stresses, strains and fluid flow. Therefore experimental techniques that permit full-sample observation of the deformation and flow are required.

This presentation will cover recent progress in using neutron diffraction and imaging (radiography and tomography) with in-situ experiments to characterise deformation mechanisms in rocks at different scales as well as to investigate the coupling between mechanical deformation and the evolution of the hydraulic properties of rocks. The reasons for using neutrons for these studies are two-fold: (i) neutrons can penetrate the metals used in pressure containment vessels, so enable “in-situ” measurements of samples under pertinent confining pressures (10’s MPa); (ii) sensitivity to hydrogen, which provides a highly sensitive measurement of water distributions and movements in bulk rock samples plus the possibility to exploit H_2O/D_2O contrast. Scanning neutron diffraction is used to map strains in the crystalline rock grains, which can potentially provide information on force/stress heterogeneity. A new experimental set-up and recent results from this work will be presented. In another project, neutron imaging is used to follow the 3D structural evolution of samples undergoing deformation, in-situ in the imaging set-up. 4D image analysis enables the deformation field and evolving heterogeneity to be characterized from the time-lapse images. This deformation analysis is linked to imaging of fluid flow through the samples at different stages of deformation with the ultimate aim to characterise the coupled hydro-mechanical processes.

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