

Processing of Milk: Drying and Pressure

Andrew Jackson¹, Duncan McGillivray², Jitendra Mata², John White²

¹University of Maryland, GAITHERSBURG, United States of America

²The Australian National University, CANBERRA, Australia

Approximately a third of the ten billion litres of milk produced in Australia each year is processed into powdered products. High protein content powders are one such type of product. These powders differ from skim milk powder in that the protein content is much higher (~80% by mass) and milk components such as lactose have been removed.

Small angle scattering (neutron and x-ray) and ultra-small angle neutron scattering (USANS) have been employed to examine the structure of these powders at varying degrees of moistness and their reconstituted solutions.

As part of these studies we have, in addition to examining the effects of drying, considered the effects of high pressure (HP) treatment. This is currently a topic of research interest, driven primarily by industrial concerns where HP is investigated as an alternative or supplement to heat treatment. High pressures have been shown to change the properties of milks, and lead to different outcomes in the production of dairy products, which are poorly understood.

The combination of neutron and x-ray scattering over a wide range of wavevector has allowed us to develop a model that fits both the dry and wet scattering data giving us insight to the effects of drying and high pressure treatment on the nanostructure of milk.

Spontaneous Self-assembly and Equilibrium Kinetics of Polymeric Micelles as seen by Time Resolved Small Angle Scattering

Reidar Lund¹, Lutz Willner², Jörg Stellbrink², Dieter Richter², Juan Colmenero¹, Peter Lindner³

¹Donostia International Physics Center, SAN SEBASTIÁN, Spain

²IFF, Forschungszentrum Jülich, JÜLICH, Germany

³Institute Laue Langevin, GRENOBLE, France

Driven by minimalization of interfacial free energy, block copolymers spontaneously self-assemble to form polymeric micelles in selective solvents, i.e. solvents that are poor for one block but good for the other. Extensive structural investigations using Small Angle Neutron Scattering (SANS) have shown that the micellar structures formed are reproducible and uniquely defined in terms of size and aggregation number [1]. Using a novel Time Resolved SANS technique in combination with a deuterium/hydrogen labelling we find that the equilibrium kinetics of such micelles is dominated by single unimer exchange. This exchange is characterized by very long time scales ranging from virtually infinity to minutes depending on the interfacial tension. In contrast to the theoretically predicted single exponential decay, data exhibit a very broad relaxation pattern which can be accurately described by a logarithmical time dependence [2, 3]. We attribute this behaviour to a dynamical coupling between the chains in the core arising from the confinement. These results in an increased cooperativity in the expulsion process that qualitatively can be understood in terms of “hierarchical constrained dynamics” that predicts a logarithmic relaxation function [4]. In order to further elaborate the influence of chain interactions and the cooperativity in the core, we have also performed measurements of triblock copolymers and compared to the diblock micelles having the same overall micellar characteristics. The results seem to indicate that chain topological interactions are responsible for the logarithmical relaxation [5].

In this presentation we will focus on the results from the equilibrium kinetics, discuss which factors control the kinetics and propose a new mechanism for the expulsion process. Implications of this work will be discussed, in view of the very slow time scales, in relation to the equilibrium properties of the micelles. The latter aspect will be highlighted by some recent results from measurements of the kinetics of self-assembly starting from a homogenous solution of unimers.

[1] Lund R, Willner L, Stellbrink, J, Radulescu, A and Richter D *Macromolecules* 37 (26): 9984-9993 (2004)

[2] Lund R, Willner L, Stellbrink, J, Richter D, Lindner, P. *Phys. Rev Lett.* 96 (6): 068302 (2006)

[3] Lund R, Willner L, Richter D, Dormidontova EE *Macromolecules* 39 (13): 4566-4575 (2006)

[4] Brey, J.J. and Prados, A. *Phys. Rev. E.* 63(2): 021108 (2001)

[5] Lund, R; Willner, L.; Richter, D.; Iatrou, H.; Hadijichristidis, N. and Lindner, P. *J. Appl. Cryst. Accepted*

Scattering from Polymer Networks under Elongational Strain

Carsten Svaneborg¹, R. Everaers², G.S. Grest³

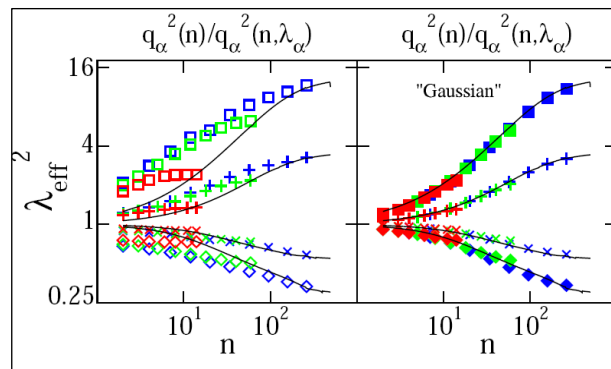
¹University of Aarhus, ÅRHUS C, Denmark

²MPI for complex systems, DRESDEN, Germany

³Sandia National Laboratories, ALBUQUERQUE, United States of America

The microscopic origin of the macroscopic elastic properties of polymeric materials is of great interest. Computer simulations are a convenient tool as they provide simultaneous access to micro and macro observables, can be used to validate the analysis of experimental data, and is applied to well characterized model networks.

The elastic properties can be predicted from the knowledge of conformational response to strain. [1] These microscopic deformations shows a non-trivial dependence on length scale: at large length scales, the response is affine, while at short length scales it is independent of strain. The cross-over is given by the tube diameter. Microscopic deformations are easily obtained from



simulations, but not from experiment. The ratio of strained to unstrained radii of gyration provides a measure of microscopic deformations, but necessitates the preparation and study of multiple comparable systems with varying label length. However, by performing just one experiment on a single system with long labeled chains at various strains, a measure analogous microscopic deformation can be obtained through an inversion procedure of the measured form factors [2].

The figure shows the microscopic deformations obtained by inverting the scattering of three different label length for two strains (2 and 4) for the simulation (left) and for equivalent Gaussian model chains (right). The source of non-Gaussian statistics in these dense networks of flexible chains remains open see e.g. [3].

The inversion provides proof-of-concept that macroscopic stress-strain behaviour can be obtained directly from scattering data from strained polymer networks.

C. Svaneborg, R. Everaers, G.S. Grest, Phys.Rev.Lett. 2004, 93, 257801; Polymer 2005, 46, 4283.

C. Svaneborg, R. Everaers, G.S. Grest, Europhysics Letters 2005, 72, 760.

J.P Witmer, H. Mayer, J. Baschnagel, A. Johner, S. Obukhov, L. Mattioni, M. Müller, A. N. Semenov Phys. Rev. Lett., 93 (2004) 147801.

Dynamic and Structural Behaviour of Microemulsion Polymer Mixtures

Tinka Spehr
I.L.L., GRENOBLE, France

The ternary microemulsion consisting of water, decane (or toluene) as oil and the anionic surfactant AOT forms a stable droplet microemulsion over a wide range of compositions. Spherical water droplets surrounded by a monolayer of AOT molecules are dispersed in a continuous oil matrix. Size and density of the droplets are independently tunable. The addition of a suited amphiphilic triblock copolymer leads to the interconnection of the droplets. The structural and dynamical behaviour of this model system for a transiently linked network is investigated with different Neutron Scattering Techniques.

Small-Angle-Scattering shows increasing ordering of the droplets with increasing polymer concentration. Structure factors and form factors are extracted.

Time-of-Flight and Backscattering measurements on pure microemulsions with different droplet sizes (diameters ranging from 3 to 10 nm) have been carried out to study the effect of spatial soft confinement on water. Fixed window scans show a deeper undercooling of the water confined in the smaller droplets.

Quasielastic measurements at temperatures between 300 and 250 K will be discussed. Besides the water the contribution of AOT has to be considered. The combination of spatial restriction and wall effects will be discussed.

As a next step the “softness” of the confinement is changed by addition of polymers.

The addition of polymers also changes the elastic properties of the droplet shell and consequently the shape fluctuations. This has been probed by Spin Echo [1].

[1] J. Huang, S. Milner, B. Farago, D. Richter (1987), PRL 59, 2600

Collective Acoustic Excitations in Fluids: a Critical Review of Neutron Spectra Interpretation and a New Analysis of the Dispersion Curve

Ubaldo Bafile¹, Fabrizio Barocchi², Eleonora Guarini²

¹CNR - Istituto dei Sistemi Complessi, SESTO FIORENTINO (FI), Italy

²Dip.to di Fisica, Università di Firenze, FIRENZE, Italy

The study of collective acoustic excitations in fluids, in the wave-vector range accessed by inelastic scattering of neutrons and x-rays, has been hampered by the use of a variety of criteria, often not put on well-founded bases, for the determination of the frequency and width of the Brillouin lines. We show that the $S(Q, \omega)$ models most commonly fitted to experimental spectra can be formulated within a common unifying scheme, so that the dispersion curve and the propagation Q -range of the excitations can be determined in a consistent, unambiguous way, whichever model is used. We illustrate a new, exact formula which allows for the first quantitative understanding of the dispersion curve and highlights the role of structural, thermal, and damping effects. We show that results obtained by fitting different models to $S(Q, \omega)$ spectra can be thus compared in a much more meaningful way than it has been possible so far.

A Novel Approach to Modelling Non-exponential Relaxation in Glasses and Spin Glasses

Catherine Pappas¹, Robert Cywinski², Ruth Pickup²

¹Hahn-Meitner-Institut Berlin, BERLIN, Germany

²University of Leeds, LEEDS, United Kingdom

Neutron Spin Echo (NSE) provides a model independent technique for directly probing complex glassy relaxation both in structural and magnetic glasses. Marked deviations from simple Debye relaxation are commonly found in glassy relaxation and are normally attributed to the presence of broad distributions of relaxation times. In such situations the stretched exponential or Kohlrausch relaxation function is often used to fit the experimental data, but the resulting parameters provide very little additional information about the nature of the distribution, or indeed whether the observed relaxation processes are parallel or hierarchical in character.

Such conventional relaxation functions cannot adequately describe some of our recent NSE measurements of relaxation in concentrated spin glass systems. We have therefore adopted an alternative approach based upon a rigorous probabilistic model developed by Weron [1]. The Weron model [2] can distinguish between parallel and hierarchical relaxation by considering an ‘interaction’ between the relaxing entity and its surrounding environment. The strength of this interaction is introduced by the “Weron” relaxation function through one additional parameter. Conveniently, the Weron function embodies both the exponential and stretched exponential forms of relaxation as special cases, and both can be recovered as the interaction parameter reduces to zero.

[1] R.M. Pickup, R. Cywinski, C. Pappas and B. Farago, ILL Annual Report, p56 (2005)

[2] K.Weron, J. Phys.: Condens. Matter 3, 915, (1991)

The Structure of Liquid Tellurium based Alloys used in DVDs and PC-RAMs of the Future

Jean-Pier Gaspard¹, Vanessa Coulet², Christophe Bichara³, Matthias Wuttig⁴, Christoph Steimer⁴, Julia Steiner⁴, Wojciech Welnick⁴, Brigitte Beuneu⁵

¹ULg, SART-TILMAN, Belgium

²TECSEN Laboratory, MARSEILLE, France

³CRMEN, MARSEILLE, France

⁴RWTH, AACHEN, Germany

⁵Laboratoire Leon Brillouin, GIF-SUR-YVETTE, France

The structure of a set of 13 liquid ternary tellurium alloys has been studied by neutron scattering ($\lambda = 0.7 \text{ \AA}$) on the 7C2 diffuse diffractometer of the LLB, Saclay. The local environment is quantified by the ratio of the heights of the first two peaks of the total scattering function $S(q)$. A characteristic change of $S(q)$ with the average number of valence electrons is found, together with a secondary effect of the atomic substitution within the same group of the periodic system. For average valence electron numbers between 4.0 and 4.25 tetrahedral local order predominates, while larger valence electron numbers induce a transition to octahedral order. We found an interesting correlation between the structure factor $S(q)$ and the phase change ability of the materials: all alloys which can be successfully used as phase change materials display an octahedral atomic arrangement in the liquid phase.

Comparison of the Liquid Structure of Carbondisulfide and Carbondioxide

Joerg Neuefeind

Oak Ridge National Laboratory, OAK RIDGE (TN), United States of America

Combination of neutron scattering data and isotopic substitution and X-ray scattering data provides direct information on the fluid structure at the partial pair distribution level. While both liquid CS₂ and CO₂ are well studied systems, earlier studies generally interpret X-ray and neutron data separately, often at unique state points in temperature and density. We measured the neutron structure factor of ¹²C and ¹³C labeled CS₂ and CO₂ as well as the X-ray structure factors of those systems. CO₂ was investigated close to the critical temperature which allows for easy variation of the density of the system. One state point was chosen such that the molecular density of CO₂ is identical to the density of CS₂ under normal liquid conditions (~300 K, 0.1 MPa), which allows a meaningful comparison of both structures. Results from scattering experiments at ILL, HASYLAB and ESRF will be presented together with results from MD simulations of these systems.

Short-range Charge Ordering in $\text{Ho}_{0.1}\text{Sr}_{0.9}\text{CoO}_{3-x}$ ($0.15 = x = 0.49$)

Marisa Medarde Barragan¹, Sabine Streule², Andrei Podlesnyak², Ekaterina Pomjakushina², Kazimierz Conder³, Sergei Kazakov⁴, Janusz Karpinski⁴, Joel Mesot²

¹Paul Scherrer Institut, VILLIGEN, Switzerland

²Lab. for Neutron Scattering, ETHZ & PSI, 5232 VILLIGEN PSI, Switzerland

³Lab. for Developments and Methods, PSI, VILLIGEN, Switzerland

⁴Laboratory for Solid State Physics ETHZ, ZURICH, Switzerland

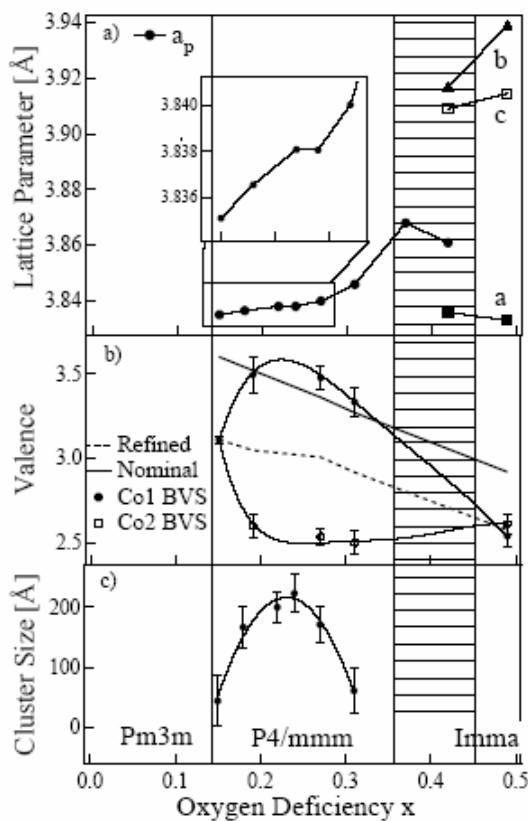
In this study we report high resolution neutron powder diffraction data of the Co perovskite series $\text{Ho}_{0.1}\text{Sr}_{0.9}\text{CoO}_{3-x}$ ($0.15 \leq x \leq 0.49$) that clearly show the existence of a nearly complete $\text{Co}^{3+} / \text{Co}^{4+}$ charge ordering for compositions close to $x = 0.23$. [1] The charge-ordering pattern is characterized by a structural commensurate modulation, which can be described with the propagation vector $\mathbf{q}_{\text{CO}} = (0 \ 0 \ \frac{1}{2})$ with respect to the cubic perovskite cell $Pm\bar{3}m$. The signature of the charge-ordered state is observed within a broad compositional range ($0.19 \leq x \leq 0.31$), although the size of the charge-ordered clusters decreases from 250 Å ($x = 0.27$) to 50 Å ($x = 0.15, 0.31$). Surprisingly, the difference δ between the bond valence sums for the Co^{3+} and Co^{4+} sites is very close to $1 e^-$ (see Fig. 1b). This observation contrasts with the situation described for the vast majority of charge-ordered oxides, where much weaker charge redistributions are

usually reported ($0.1e^- \leq \delta \leq 0.3e^-$).

We attribute this astonishing behaviour to the one-dimensional character of the associated distortion pattern, whose elastic stabilization is eased with respect to the 3D arrays reported for other charge-ordered perovskite oxides. Also, we believe that the non-existence of long-range charge order in this system may be due to the competition between the ordering of the oxygen vacancies and that of the $\text{Co}^{3+} / \text{Co}^{4+}$ species, which, due to the Ho doping, are expected to happen at different compositions ($x = 0.25$ and $x = 0.20$, respectively).

[1] S. Streule et al. PRB 73, 024423 (2006).

Figure 1. Evolution of a) the cell parameters, b) the bond valence sums and c) the cluster size of the charge-ordered domains along the $\text{Ho}_{0.1}\text{Sr}_{0.9}\text{CoO}_{3-x}$ series.



Supercells, Structural Transitions and Magnetic Properties of Cobalt based Perovskites

Chris Knee¹, Fredrik Lindberg², Gunnar Svensson², Peter Svedlindh³, Sten Eriksson⁴, Lars Börjesson⁴, Peter Hickey⁵, Mark Weller⁵, Paul Henry⁶

¹Gothenburg University, GÖTEBORG, Sweden

²Stockholm University, STOCKHOLM, Sweden

³Uppsala University, UPPSALA, Sweden

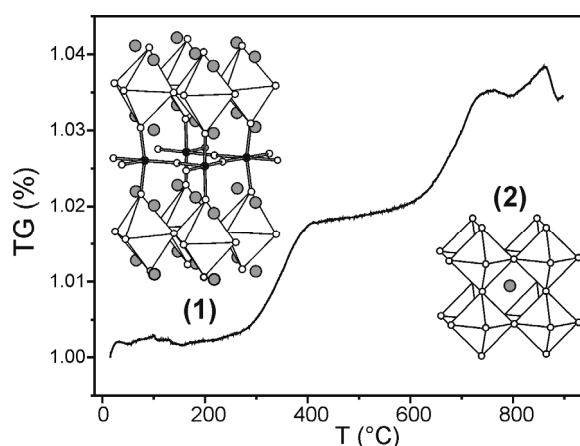
⁴Chalmers University, GÖTEBORG, Sweden

⁵University of Southampton, SOUTHAMPTON, United Kingdom

⁶Institut Laue Langevin, GRENOBLE, France

Cobalt based perovskites have been the focus of significant research efforts based on their varied properties including spin transition induced metal insulator behaviour in LaCoO_3 and magnetoresistance effects in $\text{LnBaCo}_2\text{O}_{5.4}$ ($\text{Ln} = \text{Eu}, \text{Gd}$). Recently, interest has also focused on oxygen deficient systems of the form $\text{Ln}_{1-x}\text{Sr}_x\text{CoO}_{3-\delta}$ in terms of potential applications for fuel cells.

The sensitivity of neutron diffraction to the ordering of oxygen vacancies, and subtle displacements in the oxygen lattice, which both lead to new diffraction peaks, makes it a vital tool for the characterisation of these materials. Furthermore, the technique allows magnetic order to be investigated. Here, I will report on variable temperature NPD studies of two cobalt systems of interest: i) $\text{Sr}_{1-x}\text{Bi}_x\text{CoO}_{3-y}$ ($0.1 \leq x \leq 0.2$) supercell perovskites and ii) the Ruddlesden-Popper phase $\text{Gd}_2\text{SrCo}_2\text{O}_7$.



i) The as-prepared $\text{Sr}_{1-x}\text{Bi}_x\text{CoO}_{3-y}$ compounds adopt a tetragonal ($I4/mmm$) supercell structure, with $a \approx 2a_p$, $c \approx 4a_p$, based on alternating layers of CoO_6 octahedra and CoO_{6-x} units, see (1) in the figure. On oxygen annealing the supercell collapses to a simple cubic ($Pm-3m$) perovskite, (2), and the G-type antiferromagnetic order displayed by the as-prepared samples is lost.

ii) RT neutron diffraction reveals that the structure of $\text{Gd}_2\text{SrCo}_2\text{O}_7$ is not the ideal $I4/mmm$ symmetry previously thought but instead a PA_2/mnm description based on correlated tilts of the CoO_6 octahedral bi-layers is favoured. A structural transition at $T \approx 580$ K is characterised by a clear reduction of unit cell symmetry to orthorhombic and an axial elongation of the CoO_6 octahedra; this behaviour is attributed to a spin crossover of the cobalt (III) ions, most likely from an intermediate to a high spin configuration.

Electron microscopy, magnetisation, and TGA/DSC results will also be presented to provide a complete picture of the interplay between cobalt valence, spin state, and structure.

Quantitative Texture Analysis of Deformed Natural Quartz Vein from the Torridon Area of NW Scotland with Neutron Diffraction Data

Husin Sitepu¹, Ulf Garbe², Husin Sitepu¹, Heinz-Gunter Brokmeier², Richard Law³

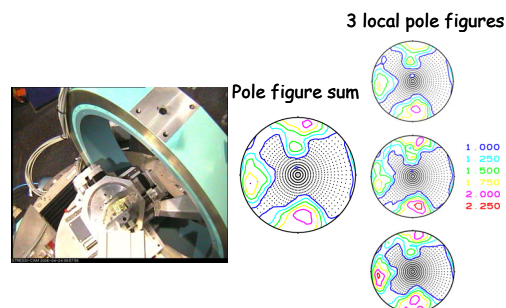
¹Prince Sultan University, RIYADH, Saudi Arabia

²GKSS-Research Center, Max-Planck-Str., GEESTAHAHT, Germany

³Department of Geosciences, Virginia Tech, BLACKSBURG, United States of America

X-ray texture goniometry and electron backscattered diffraction (EBSD) methods were originally used to measure pole figures of deformed quartz vein from Torridon area of NW Scotland and the Cambrian quartz mylonite; Stack of Glencoul, Assynt area of Moine thrust zone, NW Scotland. The results showed that individual positions on the c-axis fabric skeleton are related by a common $\langle a \rangle$ direction which is coincidence with this dominant a-axis point maximum. Thus, the crystallographic fabrics strongly support the bulk simple shear kinematic framework indicated by shear zone geometry. The crystal lattice preferred crystallographic orientation results of Stack of Glencoul sample obtained from the EBSD are consistent with co-axial strain paths. The EBSD derived lattice preferred orientation was then used to predict elastic parameters for Cambrian quartz mylonite, from which 3D seismic properties were derived.

In the present study, pole-figures of (110), (021), (111), (021), (112), (211) and (113) were measured using the STRESS-SPEC material-science neutron diffractometer at FRM-II in Garching, Germany. The bulk texture obtained from neutron diffraction, which is a very useful tool to study the bulk texture of large sample volume non-destructively because neutrons have small absorption coefficients for most materials, will be described.



Spin Correlations in Frustrated Square Lattices

Markos Skoulatos

University of Liverpool, LIVERPOOL, United Kingdom

The new frustrated square-lattice systems, $\text{Pb}_2\text{VO}(\text{PO}_4)_2$ [1] and $\text{SrZnVO}(\text{PO}_4)_2$, have been investigated using polarised neutron scattering, and these studies on powdered samples have determined the nature of the exchange interactions and the magnetic ordering for these novel quantum magnets. By employing three-dimensional polarisation analysis on the neutron spectrometers D7 and IN20 at the ILL it was possible to isolate the purely magnetic signal. Quantum order from disorder occurs at low temperature, and the ground state observed below the Néel temperature ($T_N \sim 3.5$ K and 2.7 K respectively for the Pb and SrZn compounds) is a collinear antiferromagnet. The reduced ordered moment and the coexistence of diffuse magnetic scattering down to our base temperature, $T \sim 1.5$ K, indicates the presence of considerable quantum disorder at low temperature. At room temperature there are no magnetic correlations and it is possible to model the scattering with the V^{4+} magnetic form factor. However, at $T \sim 20$ K and 35K respectively, a temperature well into the paramagnetic phase, magnetic correlations are observed, and these spin correlations have been modelled using a high-temperature series expansion. Ferromagnetic nearest-neighbour exchange J_1 and antiferromagnetic next-nearest-neighbour exchange J_2 are obtained, and this is of particular interest theoretically, since it corresponds to a new region of the J_1 - J_2 phase diagram [2].

[1] E.E. Kaul, H. Rosner, N. Shannon, R.V. Shpanchenko and C. Geibel, *J. Magn. Mater.* 272-276, 922 (2004).

[2] N. Shannon, T. Momoi and P. Sindzingre, *Phys. Rev. Lett.* 96, 027213 (2006).

A Cold Neutron Chopper Spectrometer for the ESS Long-pulse Target Station

Kim Lefmann¹, Helmut Schober², Kaspar Hewitt Klenø³, Ferenc Mezei⁴

¹Risø National Lab., Techn. Univ. Denmark, ROSKILDE, Denmark

²Institut Laue-Langevin, GRENOBLE, France

³Niels Bohr Institute, Univ. Copenhagen, COPENHAGEN, Denmark

⁴Hahn-Meitner Institut, BERLIN, Germany

The current plans for the European Spallation Source (ESS) has spawned much work on novel instrument design optimized for long-pulsed sources. We here present detailed design and analysis of a cold neutron chopper spectrometer, similar to IN5 at ILL, and optimized to run at incident wavelengths of 4-6 Å. The spectrometer has primary and secondary flight paths of 100 m and 4 m, respectively. With this design, the energy resolution of the primary and secondary spectrometers are matched, when the full 2 ms pulse is used. The spectrometer uses a wavelength multiplication scheme, where up to 11 short pulses of different wavelengths are selected within each frame, every 5 (10) ms. The wavelength difference between pulses is 0.2 (0.4) Å. The use of the full pulse, wavelength multiplication, and guide optimization yield a performance gain factor of more than 200 over the present IN5 spectrometer. Virtual experiments show that the resolution is very clean and well described by standard equations.

TOF Reflectometer Utilizing a Thermal Neutron Beam

George Apostolopoulos, K Mergia, A. Salevris, S Messoloras
NCSR Demokritos, AG. PARASKEVI ATTIKIS, Greece

In this paper we report on the main characteristics of a Time-Of-Flight reflectometer utilizing a neutron thermal beam at the Greek Research Reactor GRR-1. The main purpose of the instrument is the study of oxidization and diffusion phenomena in low dimensional systems and surface phenomena in solids and liquids. The instrument has been designed in order to allow flexible choice of wavelength range and resolution. Also the angle of the incident beam can vary in order to allow the study of liquid samples.

Monte Carlo Simulations for the New EIGER Spectrometer at PSI

Uwe Filges¹, Henrik M. Rønnow², Jonas O. Birk³

¹Paul Scherrer Institut, VILLIGEN PSI, Switzerland

²École Polytechnique Fédérale de Lausanne, LAUSANNE, Switzerland

³University of Copenhagen, COPENHAGEN, Denmark

Presently a new spectrometer for Enhanced Intensity and Greater Energy Range (EIGER) is under construction at PSI. It combines a horizontal focusing guide with virtual source, a large doubly focusing monochromator and a novel type of back end for Continuous Angle Multiple Energy Analysis (CAMEA).

Extensive Monte Carlo simulations with MCNPX and McStas were performed in order to find the optimal EIGER design. The optimisation was focused on the signal to noise ratio. Part one of the instrument design was a comprehensive simulation of the EIGER beam line including the SINQ target, the water scatterer and the neutron beam channel R82.

The focusing guide with the virtual source at the end of the guide has been installed and in 2006 the first neutron flux measurements were carried out. The comparison between measurements and simulations shows a very good agreement. Part two of the optimisation process was the design of the compact EIGER monochromator shielding. The key difficulties were to eliminate efficiently very fast neutrons (> 1 MeV) and to minimise the secondary neutron flux inside the monochromator shielding. In this paper the concept of the monochromator shielding design will be presented.

Neutron Protein Crystallography at the Institut Laue Langevin

Matthew Blakeley
Institut Laue Langevin, GRENOBLE, France

The neutron Laue diffractometer LADI is dedicated to neutron protein crystallography at high-resolution (1.5Å – 2.5Å) and is used to study key hydrogen atoms and water structure in protein single crystal structures. The instrument was originally optimized for data collection from medium size proteins (~30kDa) at room temperature. However, thanks to the ILL/EMBL/IBS deuteration laboratory, the production of fully deuterated proteins has now become routine so that it is possible to use much smaller crystal volumes and/or address much larger unit-cell projects (>150Å). Furthermore, through protocols developed for the successful cryo-cooling of large protein crystals data can also be collected at cryo-temperatures, promising to open new areas of research.

As a first step in a broader project that aims to 1) make neutron protein crystallography more accessible to the structural biology community, 2) extend the size and complexity of systems that can be studied and 3) maintain our competitiveness with diffractometers coming on-line at spallation sources, an upgraded neutron Laue diffractometer - LADI-III - has been designed, constructed and installed. Based on the design of VIVALDI (LADI-II), modifications to the detector design and readout system have been incorporated so that a miniaturized reading head located inside the drum scans the image-plate. From comparisons of neutron detection efficiency with VIVALDI, the transferral of the image-plates and readout system internally provides a 3-fold gain in neutron detection compared to LADI. Furthermore, in order to help reduce the background and the number of spatially overlapped reflections, the dimensions of the drum have been increased and the entire detector height can be adjusted to allow for relocation to a higher intensity beam, providing yet further gains. Current projects aim to address questions concerning enzymatic mechanism, ligand-binding interactions, solvent effects, structure dynamics and their implications. Some examples of recent results will be presented.