BOOK OF ABSTRACTS

International Seminar NEUTRONS AND SYNCHROTRON RADIATION IN INVESTIGATIONS OF CONDENSED MATTER

October 12-13, 2021

ONLINE FORMAT

Adam Mickiewicz University Poznań
Faculty of Physics

FLNP

65 Joint Institute for Nuclear Research 1956

SOLARIS Narodowe Centrum Promieniowania Synchrotronowego

Welcome to International Seminar

NEUTRONS AND SYNCHROTRON RADIATION IN INVESTIGATIONS OF CONDENSED MATTER

Dear Colleagues,

We would like to thank all of you for your participation at the conference. It is a great pleasure for us to meet you during the next edition of our Seminar.

The current edition of the Seminar was organized thanks to the cooperation of Institutions such as: Frank Laboratory of Neutron Physics in Joint Institute for Nuclear Research in Dubna (Russia), Faculty of Physics in Adam Mickiewicz University in Poznan (Poland) and National Synchrotron Radiation Centre SOLARIS in Jagiellonian University in Krakow (Poland).

We are proud to announce that the current seminar has outstanding scientific program which consists of 23 invited talks.

We do hope you will find the Seminar interesting!

Maciej Kozak (AMU Poland/UJ Poland) – chairman

Dorota Chudoba (AMU Poland/JINR Russia) – co-chairman

PROGRAM

Tuesday 12.10

09:00 **Opening**
Maciej Kozak (AMU/NCPS Solaris, UJ, Poland)

09:10 Opening
Wojciech Nawrocik (AMU, Poland)/ **Jan Wąsicki** (AMU, Poland)

Chair: Wojciech Nawrocik

10:40 - 10:50 Coffee break

Chair: Denis P. Kozlenko

12:50 - 14:30 Lunch

Chair: Norbert Kucerka

Wednesday 13.10

Chair: Jan Wąsicki

9:00 - 9:40 Development of the Conceptual Design of a New Neutron Source at JINR 18
Valery Shvetsov (FLNP JINR, Russia)

9:40 -10:20 SOLARIS synchrotron performance and future plans..... 20
Adrianna Wawrzyniak (NCPS Solaris, UJ, Poland)

Chair: Timur Tropin

10:20 - 10:30 Coffee break

10:30 - 11:00 Dynamic properties of glass of disordered phases..... 21
Ewa Juszyńska-Gałązka (IFJ PAN, Poland)

11:00 - 11:30 Solution scattering and characterization of selected multimeric complexes 22
Michał Taube (UAM, Poland)

11:30 - 12:00 Selected properties of Ga-substituted Fe_3O_4 nanoparticles with potential biomedical applications 23
Katarzyna Rećko (UwB, Poland)

12:00 - 12:30 Structure of magnetic nanoparticles in bulk and at interfaces by neutron scattering 24
Viktor Petrenko (BCMaterials, Spain)

12:30 - 14:30 Lunch

Chair: Marek Stankiewicz

14:30 - 15:00 Motion of a Membrane Enzyme as Seen by SANS 25
Anne Martell (ILL, France)

15:00 - 15:30 High-pressure effect on crystal and magnetic structure of complex nanostructured oxides 26
Nadezhda Belozerova (FLNP JINR, Russia)

15:30 - 16:00 Reversible control of magnetism in FeRh thin films 28
Denes Nagy (WRCP Hungary)

16:00 - 16:15 Hemocyanin from the great pond snail Lymnaeastagnalis – protein with unique structure and anticancer activity 29
Kamil Szpatkowski (IBC PAS, Poland)

16:15 - 16:30 Formation of micelle-polymer complexes in the bulk of surfactant solution and interface of polymer brush system 30
Oleksandr Artykulnyi (FLNP JINR, Russia)

16:30-16:45 **Closing**

Current status of National Synchrotron Radiation Centre SOLARIS

Marek Stankiewicz and SOLARIS NSRC team

SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Kraków, Poland

SOLARIS National Synchrotron Radiation Centre at Jagiellonian University (Kraków, Poland) is the first synchrotron in Central and Eastern Europe. At SOLARIS 1.5 GeV storage ring presently 4 beamlines with 8 end-stations are available for users and 4 further ones are at the construction phase. The synchrotron is open for Polish and international users. 517 scientists performed their experiments within 257 projects accepted in 7 open calls since 2018. During the lecture the current status of SOLARIS NSRC and future plans will be presented.

Hard and Soft Condensed Matter Studies at the IBR-2 Pulsed Reactor

Norbert Kučerka

Frank Laboratory of Neutron Physics Joint Institute for Nuclear Research, Dubna, Russia

Each Laboratory has its own prehistory and destiny. The establishment of Frank Laboratory of Neutron Physics is connected closely to the first and only pulsed reactor in the world. The economic advantages of IBR-2 reactor allow to run the facility for many past and future years. The examples of possible scientific investigations will be presented from a wide range of condensed matter research, not forgetting the field of soft matter and life science.

Atomic and Spin Dynamics in Condensed Matter by Neutron Scattering with Crystal Spectrometers

Alexandre IVANOV

Institut Laue-Langevin, Grenoble, France

The crystal neutron spectrometers have strongly profited from now routinely used two-dimensionally focusing monochromators and analysers with variable and remotely controlled curvatures. The brightness of a measured ($\mathbf{Q}$,ω) pixel may be increased with these high-precision mechanical devices by a factor of more than 100. Several multi-analyser (multi-pixel) schemes have been proposed and designed with a varied progress. Promising results have been achieved in studies of polycrystalline materials using large focusing crystal surfaces that permit registration of scattered neutrons in considerable solid angle. Several examples of recently collected data will be presented. Further efforts on the optimisation and multiplexing of neutron crystal spectrometers will be indicated.

SMALL ANGLE NEUTORN SCATTERING & HARD MATTER DOWN UNDER

A.Sokolova

Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights, New South Wales, 2234, Australia

Australian Nuclear Science and Technology Organization (ANSTO) successfully operates two small angle neutron scattering instruments, Quokka [1] and Bilby [2], and an ultra-small angle scattering instrument Kookaburra [3]. Quokka is a monochromatic instrument equipped with a polarizer and focusing lenses. Bilby is Time-of-Flight instrument having a monochromatic option too. The design of Bilby opens the possibility to vary wavelength resolution in the wide range (from 4% to 30%) satisfying various scientists' requirements. Two arrays of position-sensitive detectors in combination with utilizing of wide wavelength range (from ~2Å to ~20Å) provide the capability to collect scattering data of wide angular range without changing the experimental set-up. Kookaburra's design is based on a Bonse-Hart principle. Altogether, three instruments can cover Q (momentum of transfer) range from 1.8 x 10-5 to 1.8 Å-1, opening the possibility to study a massive range of materials.

Each instrument has a range of sample environments allowing to collect data from the samples in the magnetic field, wide range of temperature, at the shear, and so on.

This presentation will focus on results obtained recently on the hard matter systems, like metals, coals, superconductors, and single crystal skyrmion systems. The main aim of this talk is to demonstrate the capabilities of our facilities indicating that we are open to collaboration.

References

[1] "QUOKKA, the pinhole small-angle neutron scattering instrument at the OPAL Research Reactor, Australia: design, performance, operation and scientific highlights " Wood, K et al, J. Appl. Crystallography , 51(2), p.294-314 (2018)

[2] "Performance and characteristics of the BILBY time-of-flight small-angle neutron scattering instrument", Sokolova A. et al, J. Appl. Crystlography, 52, p.1-12 (2019)

[3] "Design and performance of the variable-wavelength Bonse–Hart ultra-small-angle neutron scattering diffractometer KOOKABURRA at ANSTO" Rehm C. at al, J. Appl. Crystallography, 51(1), p.1-8 (2018)

Facilities for Macromolecular Crystallography at the HZB

M. S. Weiss, T. Barthel, R. Förster, P. Fröling, C. Gless, T. Hauß, M. Hellmig, F. Lennartz, M Steffien, J.. Wollenhaupt & U. Mueller

Helmholtz-Zentrum Berlin, Macromolecular Crystallography, Albert-Einstein-Str. 15, D-12489 Berlin, Germany

The Macromolecular Crystallography (MX) group at the Helmholtz-Zentrum Berlin (HZB) has been in operation since 2003. Since then, three state-of-the-art synchrotron beam lines (BL14.1-3) for MX have been built up on a 7T-wavelength shifter source [1-3]. Currently, the three beam lines represent the most productive MX-stations in Germany, with almost 4000 PDB depositions. BLs14.1 and 14.2 are energy tuneable in the range 5.5-15.5 keV, while BL14.3 is a fixed-energy side station (13.8 keV). All three beam lines are equipped with state-of-the-art PILATUS-detectors. Beam lines BL14.1 and BL14.2 are in regular user operation providing about 200 beam days per year and about 600 user shifts to approximately 100 research groups across Europe. BL14.3 has been equipped with a HC1 crystal dehydration device and a REX nozzle changer and has its role as an experimental station for innovative experiments. Additional user facilities include office space adjacent to the beam lines, a sample preparation laboratory, a biology laboratory (safety level 1) and high-end computing resources. In the talk, a summary on the experimental possibilities of the beam lines and the provided ancillary equipment for the user community will be given.

[1] U. Heinemann, K. Büssow, U. Mueller & P. Umbach (2003). Acc. Chem. Res. 36, 157-163.

[2] U. Mueller, N. Darowski, M. R. Fuchs, R. Förster, M. Hellmig, K. S. Paithankar, S. Pühringer, M. Steffien, G. Zocher & M. S. Weiss (2012). J. Synchr. Rad. 19, 442-449.

[3] U. Mueller, R. Förster, M. Hellmig, F. Huschmann, A. Kastner, P. Malecki, S. Pühringer, M. Röwer, K. Sparta, M. Steffien, M. Ühlein, P. Wilk & M. S. Weiss (2015). Eur. Phys. J. Plus 130, 141-150.

Soft matter studied by Polish neutron scattering community – a subjective view plus examples from own workspace

Wojciech Zając

Institute of Nuclear Physics Polish Academy of Sciences

The landscape of soft matter research with the help of neutron scattering methods extends far beyond what one would expect, and extends from e.g. the study of lipid bilayers (including their interaction with nanoparticles) to, for example,*Glass Transition in Rice Pasta as Observed by Combined Neutron Scattering and Time-Domain NMR* [1]. A very short outline will be presented of what Polish soft matter researchers do with neutrons.

Recently, more and more people are looking into the properties of soft matter, such as liquid crystals, subjected to spatial confinement of several nanometer. This is of interest not only to those engineering high-resolution displays or targeted drug delivery vehicles. With the use of Small Angle Scattering (SANS) and Small Angle X-ray Scattering we managed to estimate the thickness of so-called paranematic layer of a liquid crystal, that forms at the inner walls of nanopores filled with a liquid crystal [2], as well as pinpoint the onset of short-range order of such molecules when they have enough steric conditions. If not, additional free volume develops with the effect upon vibrational properties as seen by Inelastic Neutron Scattering. SANS and SAXS can be combined, and aided with extensive numerical simulations to study the formation of do called gemini surfactant micelles. We managed to provide a consistent description of the phenomenon [3].

Large scale neutron facilities, such as ILL or ESS can and will be able to deliver very intense neutron beams enabling some less conventional and demanding experiments such as the ones with polarized neutrons and the analysis of polarization after scattering. This method proved unique in the characterization of residual stress of an elastomer making up a composite with a porous ceramic. This example, a pretty old one, is brought here to stimulate interest in the opportunities to be shortly offered by the European Spallation Source.

References

[1] *Polymers* **2021**, *13*(15), 2426; https://doi.org/10.3390/polym13152426

[2] E. Juszyńska-Gałązka, W. Zając, D. Soloviov, to be published

[3] K. Łudzik, S. Woloszczuk, W. Zając, et al. *Int. J. Mol. Sci.***2020**, *21*(16), 5828; https://doi.org/10.3390/ijms21165828

[4] W. Zając, A. Boczkowska et al., https://doi.org/10.1016/j.actamat.2008.08.004

Monoclinic symmetry of α-Fe_2O_3 and Cr both below and above the Neel temperature

R. Przeniosło, P. Fabrykiewicz and I. Sosnowska

Faculty of Physics, University of Warsaw, Pasteura 5, 02-097 Warsaw, Poland

High-resolution synchrotron radiation powder diffraction studies of α-Fe_2O_3 [1] and chromium [2] have been performed both below and above their Neel temperatures, T_N. The Bragg peaks of bothα-Fe_2O_3 [1] and chromium [2] observed below T_N show a hkl-dependent broadening which can be interpreted quantitatively as an indication of a lowering of the lattice symmetry. It means that the crystal structure of α-Fe_2O_3 [1] has a monoclinic symmetry instead of the trigonal symmetry of the corundum-type structure. The crystal structure of chromium [2] has also a monoclinic symmetry instead of the cubic symmetry of the bcc structure. The monoclinic symmetry of the crystal structure of bothα-Fe_2O_3 [1] and chromium [2] is also observed above T_N.

References

[1] P. Fabrykiewicz, M. Stękiel, I. Sosnowska and R. Przeniosło, *Acta Cryst* **B73**, 27 (2017).

[2] R. Przeniosło, P. Fabrykiewicz, I. Sosnowska, D.Wardecki, W.A. Sławiński, H.Y. Playford, R. Hempelmann, M. Bukowski, *Physica* **B530**, 183 (2018).

In-vacuum long-wavelength macromolecular crystallography – Experiments at the edge

Armin Wagner

Diamond Light Source, Chilton, UK

Long-wavelength or tender X-rays in the range from 2.1 to 5.9 Å (2.1 – 6 keV) cover the absorption edges of light elements of high importance in biology, such as phosphorus, sulphur, chlorine, potassium and calcium. Anomalous scattering close to their absorption edges can be probed by long-wavelength macromolecular crystallography (MX). Solving the crystallographic phase problem by single wavelength anomalous diffraction (SAD) directly in the absence of a known protein model similar to the one under investigation and without additional labelling of the protein or nucleic acid is a powerful phasing technique for macromolecular crystals. Additionally, the interpretation of anomalous difference Fourier maps calculated from data above and below these absorption edges allows to assign the identity for these elements directly without any further geometrical or biochemical evidence.

At Diamond Light Source, the long-wavelength MX beamline I23 [1] is a unique instrument covering the wavelength range from 1.1 to 5.9 Å (2.1 – 11.5 keV). The beamline differs radically from the existing well developed and established MX beamlines. To eliminate air absorption, the complete beamline is operated in vacuum, including the sample environment and the detector. Several technical challenges had to be addressed, leading to a variety of pioneering new developments, like the large in-vacuum semi-cylindrical Pilatus 12M detector, the dedicated kappa goniometer, new conductive sample mounts and an air-lock system to transfer cryogenically cooled crystals into the large vacuum end station.

Several structures have been solved using SAD phasing based on phasing information from phosphorus, sulphur, potassium, calcium, vanadium and other elements [2,3].Studies around the potassium absorption edge have provided further insight into the selectivity filter of potassium channels [4,5] and the function of the ribosome [6].An overview on the project and results from this unique facility will be presented.

[1] A. Wagner et al.*Acta Cryst.* D**72** (2016) 430.
[2] A. F. Rudolph et al.*Nat. Chem. Biol.* **15** (2019) 975.
[3] J. P. O'Donnell et al. *eLife*9 (2020) e57887.
[4] P. S. Langan et al. *Nat Commun* **9**(2018) 4540.
[5] M. Lolicatoet al. *Sci. Adv.***6 (**2020) eabc9174.
[6] A. Rozov et al. *Nat. Commun.***10**(2019) 2519.

Optical design of the SOLCRYS beamline at NSRC SOLARIS

Tomasz Kołodziej

National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, Czerwone Maki 98, 30-392 Kraków, Poland

Keywords: synchrotron radiation, beamline design, optical simulations, ray tracing

*e-mail: t.kolodziej@uj.edu.pl

SOLCRYS beamline at National Synchrotron Radiation Centre SOLARIS is one of the upcoming beamlines, dedicated to crystallographic research. The SOLCRYS beamline will be built thanks to the cooperation of the Jagiellonian University with the Joint Institute for Nuclear Research in Dubna (Russian Federation). Beamline is designed to operate in hard x-ray regime (5 – 25 keV photon energies). Since the machine is the low energy storage ring (1.5 GeV electron beam energy), so called insertion device, namely superconducting wiggler, will be used as the source of hard x-ray photon beams.

Construction of the beamline will have to meet number of technical challenges, e.g. the length of the beamline (~45 m from the source) requires extension of the experimental hall, and since this will be first hard x-ray beamline at SOLARIS, adjustment of the infrastructures (e.g. cryogenic cooling of the optics, etc.) has to be prepared.

Beamline will consist of two branches. First one (“PX” branch) will be dedicated to macromolecular crystallographic research, protein crystallography, single crystal diffraction (also under extreme conditions), etc. Second one (“SAXS” branch) will be dedicated to small-angle x-ray scattering, especially for biological samples. Two separated endstations are supposed to operate simultaneously. Different scopes are considered for the beam-sharing, including cooled fixed mask (idea similar to beamline BL14.1-3 at Bessy II, HZB [1]), or side-bounce mirror in the front-end section (outcoupling portion of the ID beam to one of the endstations).

Different specifics of the techniques exploited at two endstations call for different parameters of the beam delivered to the users, in the meaning of the flux, spot size, beam divergence and energy resolution. While at the PX branch we aim at the flux and focus, at the SAXS endstation desired shape and smallest achievable divergence of the beam is the goal. This calls for different optical layouts of two branches, regarding collimating the beam onto the monochromator for the best usage of the single crystal’s Darwin width of the reflection, and focusing the beam on the sample position. Additionally, to maximize the flux at the SAXS branch, wide bandwidth monochromator based on the multilayer optics interchangeable with standard crystal monochromator is considered.

To evaluate the performance of the whole optical setup the optical simulations (geometrical ray tracing) have to be conducted. It was done with the use of most popular codes: XOP/Shadow [2] and OASYS/ShadowOui [3]. Codes allow to model the performance of the complete beamline, from the generation of the radiation in the insertion device to the propagation of the x-ray beam through the optical system with the assumption of the realistic parameters of the elements (slope errors of the mirrors, reflectivity of the surfaces, etc.)

References:

[1] **M. Gerlach, U. Mueller and M. S. Weiss, "The MX beamlines BL14.1-3 at BESSY II",** Journal of large-scale research facilities, 2, A47 (2016)

[2] M. Sánchez del Río and R. J. Dejus. "XOP v2.4: recent developments of the x-ray optics software toolkit" SPIE proceedings 8141 (2011)

[3] L. Rebuffi, M. Sanchez del Rio, "ShadowOui: A new visual environment for X-ray optics and synchrotron beamline simulations", J. Synchrotron Rad. 23 (2016)

Geometry and resolution calculations of the new INS spectrometer at FLNP JINR

KLEPACKA M.[1,2] , Goremychkin E.A.[1] , Belushkin A.V.[1] , Chudoba D.M.[1,2]

[1]*Physics Faculty, Adam Mickiewicz University, Poland*
[2]*Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Russia*

E-mail for corresponding author: marta.klepacka@amu.edu.pl

The inverse-geometry inelastic neutron spectrometer NERA has already been operating for more than three decades and during that time has proven to be a very successful machine for broadband chemical spectroscopy with neutrons. To continue the research using the best modern technologies, the project of a new inverse-geometry inelastic neutron spectrometer has been started. New instrument will be located in the Frank Laboratory of Neutron Physics (JINR, Russia) at IBR-2 pulse reactor. Its parameters will significantly outdo the parameters of NERA spectrometer. With solid angle of 6.4 sr and resolution of the elastic line at the level of 0.55 meV the new instrument will allow to perform chemical spectroscopy with neutrons on a world-class level. Calculations of the secondary spectrometer's geometry and performance were carried out during the design phase of the project and they are presented in this work. The main concept is to place a set of HOPG analysers resembling a bell shape, on both sides of the sample position. Design and optimization of the secondary spectrometer were accomplished using Monte-Carlo ray tracing simulation software McStas and analytical methods.
Project of new INS spectrometer is supported by the Grant from the Polish Plenipotentiary in JINR, Dubna, Russia (Regulation no. 166 of 11.03.2021, article 5).

Hydrogen detection in thin films by resonant neutron reflectometry

Laura Guasco

Max Planck Institute for Solid State Research

The study of hydrogen diffusion and storage in different materials is crucial in the challenge of an actual implementation of sustainable energy sources, but also to explore the possible modification of electronic, magnetic and optical properties of the host materials. Due to high sensitivity of neutrons to hydrogen atoms, neutron scattering techniques have been successfully used for many decades. Neutron reflectometry in particular is demonstrated to be a powerful method for the study of hydrogen absorption in thin films for atomic concentrations of 5% and higher. In this talk we will show a new model-free method which allows to measure smaller (<5%) concentrations of hydrogen absorbed in situ, with smaller counting times and with a higher sensitivity. The method is based on measuring the position of the resonance formed due to the contrast between the optical potential of a layer and its neighbours. Hydrogen absorption leads to a change of this optical potential and hence to a shift of the resonance position. We will present experiments conducted on Al2O3/Nb(x)/Co(3nm)/Nb(x)/Pt(3nm) thin films demonstrating that hydrogen concentrations below 1% and absorption kinetics of few seconds can be measured using this method.

Characteristics of the relationship between amyloid-beta oligomers with Human Cystatin C

Adriana Żyła[a,b], Anne Martel[c], Michał Taube[a], Przemysław Jurczak[e], Igor Zhukov[d], Aneta Szymańska[e], Maciej Kozak[a,f]

[a]*Department of Macromolecular Physics, Faculty of Physics, Adam Mickiewicz University in Poznan, Poland*
[b]*NanoBioMedical Centre, Adam Mickiewicz University in Poznan,*
[c]*Large Scale Structures, ILL Neutrons for Society, Institute Laue-Langevin, Grenoble, France*
[d]*Department of Biophysics, Institute of Biochemistry and Biophysics, Polish Academy of Science, Warsaw*
[e]*Laboratory of Medical Chemistry, Department of Biomedical Chemistry, Faculty of Chemistry, Gdansk University, Poland,*
[f]*SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Kraków, Poland.*

* - presenting author's email: adrzyl@amu.edu.pl

The neurodegenerative diseases (Creutzfeldt-Jakob or Alzheimer's diseases, various types of amyloidosis, or Huntington's disease) are incurable, and all attempts to develop effective drugs have been unsuccessful. The investigation of intermolecular interaction based on atomic structures of amyloid β (Aß) peptides or human cystatin C (protein detected in amyloid plaques), permits an understanding of the pathological aggregation process into neurotoxic oligomers, and then amyloid plaques. Besides, it can also elucidate the possible self-defense mechanisms of the organism. Recent promising studies showed that human cystatin C (HCC) is possibly involved in the inhibition of Aß peptides aggregation into neurotoxic oligomers, the initial step of Alzheimer's disease.

Our goal was to characterize the mechanism of the Aß peptide fibrillization, in particular, fibrillization in the presence of HCC. Therefore, we started to study the interactions between native HCC and selected Aß peptides by the use of advanced biophysical methods. Our recent outcome from the combination of small-angle X-ray and neutron scattering techniques (SAXS/SANS) shed light on the possible anti-aggregation properties of HCC on selected Aβ oligomers. Our studies show that HCC probably can even depolymerize Aß 3-28 fibers, however, the Aß 1-42 fibers exhibit significant resistance. This observation can be crucial to understand the aggregation mechanism and stability of fibers on the atomic level. Therefore, it is important to characterize these binary complexes, especially to show the differences in intermolecular interactions and also to propose the structural scheme of binding between HCC and Aß peptides.

Acknowledgments

The studies were supported by a research grant 2017/27/B/ST4/00485 from the National Science Centre. AŻ acknowledge also the financial support from POWR.03.02.00-00- I032/16 from European funds.

References

[1] Sastre K et al (2004) Neur of Ag. 25(8):1033-43
[2] Choi TS et al (2017) J Am Chem Soc. 139(43):15437-15445
[3] Spodzieja et al (2017) J Mol Recognit. 30(2)

Development of the Conceptual Design of a New Neutron Source at JINR

Valery Shvetsov

Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia

JINR has a long tradition in Condensed Matter and Neutron Physics research employing neutrons from their on-site research reactors. JINR intends to stay at the forefront of this science by building the best neutrons source possible.

Neutrons are used for studying fundamental symmetries and interactions, structure and properties of nuclei, but nowadays neutrons are mostly required in investigations of condensed matter including solid states, liquids, biological systems, polymers, colloids, chemical reactions, engineering systems, etc. Moreover, extremely low energy neutrons are also a very promising tool for research in the field of particle physics and studies of fundamental interactions.

Considering the present-day tendency in neutron facility development, after 2030 only five sources will be available including three currently operating facilities: ISIS (Didcot, UK), SINQ (PSI, Villigen, Switzerland), FRM II (TU Munich, FRG), and two new sources (ESS (Lund, Sweden) and steady-state reactor PIK (PNPI NRC KI, Gatchina, Russia), both under construction with the start of operations planned for 2023-2024.

Thus, the need for a next-generation high-flux neutron source is driven by a growing interest in neutron investigations against the background of a steadily decreasing number of neutron sources in the world, as evidenced by the analysis of a specially established ESFRI “Physical Sciences and Engineering Strategy Working Group”. Such a new source will in a great extent compensate the losses of the neutron beam time in Europe and attract users that are currently served at ILL and medium-flux reactors in Germany, France and Hungary.

JINR has proposed to build a new advanced neutron source, DNS-IV (Dubna Neutron Source IV-th generation), on site. In combination with modern moderators, neutron guides and neutron scattering instruments (DNS-IV) promises to become one of the best neutron sources in the world and will open unprecedented possibilities for scientists from JINR member states and worldwide for research in condensed matter physics, fundamental physics, chemistry, novel materials and life science.

DNS-IV will provide shorter neutron pulses, however containing the same number of neutrons as at European Spallation Source (ESS, to be operational in 2024). Indeed, it will be as good as ESS for low-resolution experiments and significantly outperform it for high-resolution experiments.

From the different concepts studied, a pulsed neutron reactor IBR-3 with Np-237 core was chosen for the DNS-IV project. Therefore, the pulsed neutron reactor IBR-3 with NpN fuel currently became the working project with a planned start of the DNS-IV operation is 2036-2037.
A rough cost estimate today is at about 440 M€. More exact figures are expected end of 2022 in the preliminary design stage of the project.

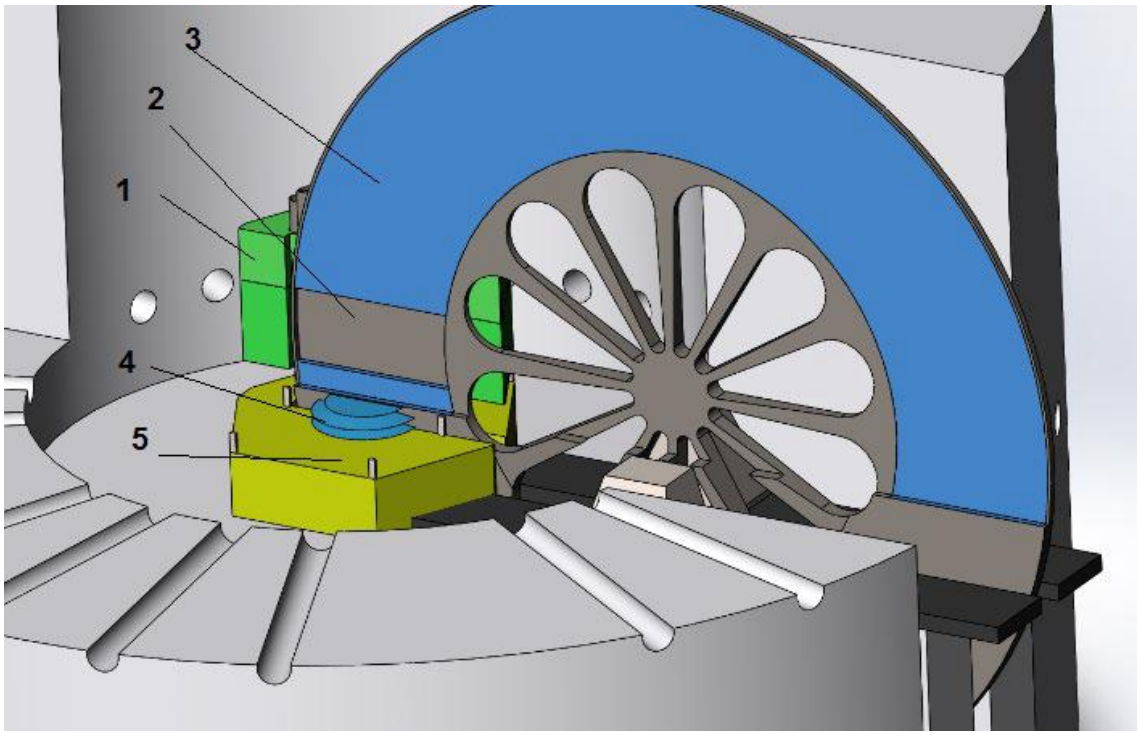

Figure : schematic view of the IBR-3: 1- reactor core reactor core, 2 - empty sector of reactivity modulator, 3 - reactivity modulator coated with titanium hydride coating, 4 - moderator, 5 - beryllium reflector.

SOLARIS synchrotron performance and future plans

Adrianna I. Wawrzyniak*

SOLARIS National Synchrotron Research Centre JU, Czerwone Maki 98, 30-392 Kraków, Poland

*adriana.wawrzyniak@uj..edu.pl

SOLARIS is a third generation light source operating since 2015 in Krakow, Poland. The project was started in 2010 as a green filed project with unique cooperation between JU and the MAX-Lab in Lund, Sweden. Between 2015 and 2018 the synchrotron as well as two beamlines were commissioned. During commissioning phases the good performance of the storage ring has been reached [1-3]. The beam optics was brought close to the design one.

Since October 2018 SOLARIS synchrotron delivers the beam to users. The storage ring is operating at an energy of 1.5 GeV in a decay mode with maximum current of 400 mA and total lifetime of 15 h [3]. Since 2018 high beam availability above 90 % was reached. In 2021, 4654 h of total beamtime was scheduled. The injection to the storage ring is done twice per day and 22h/day of beam time is declared for the users. Solaris Centre is under permanent development and new beamlines are under design and construction. In the near future also the SOLARIS experimental hall is planned to be expanded which is going parallelly with the construction of the hard X-ray beamline SOLCRYS. During the presentation the current operational status and main parameters of Solaris synchrotron as well as future perspectives will be given.

References

[1] A.I. Wawrzyniak et al, ”First Results of Solaris Synchrotron Commissioning”, IBIC2015, Melbourne, Australia, Sep 2015.

[2] A.I. Wawrzyniak, A. Kisiel, A. Marendziak et al, Proceedings of IPAC2017, WEOCA01, Copenhagen Denmark (2017), 2490.

[3] A.I. Wawrzyniak et al, “Solaris a new class of low energy and high brightness light source”, Nuclear Inst. and Methods in Physics Research, B 411, (2017) 4.

Dynamic properties of glass of disordered phases

Ewa Juszyńska-Gałązka[a,b], Wojciech Zając[a] and Dorota Chudoba[c,d]

[a]*Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Krakow, Poland*
[b]*Research Center for Thermal and Entropic Science, Graduate School of Science, Osaka University, Japan*
[c]*Frank Laboratory of Neutron Physics Joint Institute for Nuclear Research, Dubna, Russia*
[d]*Adam Mickiewicz University, Faculty of Physics, Poznan, Poland*

Polar compounds (phenyl alcohols, phenols, liquid crystals) tend to form glassy states, the properties of which depend on a cooling rate of supercooled thermodynamic phases. Structure of molecules, inter alia, through a presence or absence of specific atomic groups, or position of such groups with respect to the molecular skeleton, significantly influences the type of thermodynamic phases formed. The latter will often be partially disordered with respect to translational and/or rotational degrees of freedom, thus capable of undergoing glass transitions.

The aim of our research is to determine the physicochemical properties of glass forming organic compounds. Such compounds are also of much interest to the food, pharmaceutical or cosmetic industries, what stimulates their studies by complementary methods. In particular, amorphous forms are usually more biocompatible than crystal phases. Along this line, we embarked on the investigation of polymorphism and dynamics in various thermodynamic states that occur in these substances.

Results of infrared absorption and neutron spectroscopy, i.e., inelastic neutron scattering [1, 2] for this type of compounds, will be presented. The results of our research will be compared with the literature data for similar molecular systems [2-3].

Through Inelastic Neutron Scattering we establish vibrational dynamic of proton group and the nature of hydrogen bond. Moreover, density of states $G(\nu)$, observed in a glass of disordered phases (Debye vs. non-Debye $G(\nu)$ at small energy transfer and at helium temperature) will give information on the kind of glassy states. A combination of infrared and inelastic neutron scattering spectroscopies with the density functional theory and semi-empirical calculations was applied to propose an assignment of the vibrational spectra of chosen molecular matter compounds.

Acknowledgements

(E.J.-G.) This research was in part financed by the Plenipotentiary Representative of the Government of the Republic of Poland at JINR, Dubna within the Cooperative Project PWB / 168-12 / 2021.
The DFT calculation have been performed with help of PL-Grid Infrastructure at the ACK CYFRONET AGH in Kraków.

References

[1] I. Natkaniec, D. Chudoba, Ł. Hetmańczyk, V. Yu. Kazimirov, J. Krawczyk, I. L. Sashin and S. Zalewski,J. Phys. Conf. Ser. 554 (2014) 12.
[2] E. Juszyńska, M. Massalska-Arodź, I. Natkaniec, J. Krawczyk, Physica B 403 (2008) 109-114.
[3] E. Juszyńska-Gałązka, W. Zając, Y. Yamamura, K. Saito, N. Juruś, Phase Transit., 91 (2018) 170-185.

Solution scattering and characterization of selected multimeric complexes

Michal Taube

Adam Mickiewicz University, Poznan, Poland

Macromolecular complexes play pivotal role in almost all of the biological processes. Trough dynamic and multiple interactions they coordinate in precise manner the time, place and outcome of those processes. It is estimated that human genome encodes for more than 20000 protein coding genes. Most of the proteins in eukaryotic cell form complexes with other proteins as well as nucleic acids to perform its function. Understanding how the proteins and nucleic acids interact and form multimeric assemblies is important for the understanding basic biology. In the advent of synthetic biology knowledge how macromolecules assemble is also crucial for designing novel innovative pharmaceuticals and artificial biological machines. Many of the macromolecular complexes are dynamic in nature and too large to be study by conventional structural biology methods like X-ray crystallography or nuclear magnetic resonance. Solution scattering methods are complementary to those methods offering possibility to study dynamic, disordered and large multimeric complexes. Here we will present some recent results from our laboratory concerning structure and dynamics of protein complexes and assemblies playing role among others in RNA metabolism or amyloidogenesis.

Acknowledgments

The studies were supported by a research grant 2017/27/B/ST4/00485 from the National Science Centre (Poland).

Selected properties of Ga-substituted Fe_3O_4 nanoparticles with potential biomedical applications

Katarzyna Rećko[a], Marta Orzechowska[b], Maria Biernacka[a] Urszula Klekotka[c], Dariusz Satuła[a], Wojciech Olszewski[a], Ewa Grabowska[b], Adam Tylicki[d], Beata Kalska-Szostko[c], Dmytro Soloviov[e], A. Beskrovnyi[e], Arkadiusz Miaskowski[f], Janusz Waliszewski,[a,e] and K. Szymański[a]

[a]*Faculty of Physics, University of Bialystok, K. Ciołkowskiego 1L, 15-245 Białystok, Poland*
[b]*Doctoral School of Sciences and Natural Sciences, University of Bialystok, K. Ciołkowskiego 1K, 15-245 Białystok, Poland*
[c]*Faculty of Chemistry, University of Bialystok, K. Ciołkowskiego 1K, 15-245 Białystok, Poland*
[d]*Faculty of Biology, University of Bialystok, K. Ciołkowskiego 1J, 15-245 Białystok, Poland*
[e]*Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research Joliot-Curie 6 141980 Dubna, Moscow region, Russia*
[f]*Department of Applied Mathematics and Computer Science, University of Life Sciences in Lublin, Akademicka 13, 20-950 Lublin, Poland*

The magnetic nanoparticles have been widely used in biomedicine for drug delivery or hyperthermia [1-5]. Fe_3O_4 substituted with Co^{2+}, Ni^{2+}, Zn^{2+}or Ga^{3+}: $Ga_xFe_{3-x}O_4$ with $0 \leq x \leq 1.4$, form a group of innovative materials [6-8]. Gallium nanoferrites seem to be promising biomaterials that exhibit superparamagnetic fluctuations up to temperatures above 315 K. X-ray and neutron diffraction, transmission electron microscopy, magnetization, and Mössbauer spectroscopy studies together with calorimetric and cytotoxic tests were collected for $Ga_xFe_{3-x}O_4$synthesized by different methods. The reverse spinel structures of core and core-shell gallium ferrites have been confirmed as single phases (sg. 227: Fd-3m). The in-site occupancy preference as a function of gallium dopant is discussed. The systems have been quickly saturated and showed neglectable coercive fields while the spontaneous magnetization did not exceed 58 emu/g.$Ga_{0.6}Fe_{2.4}O_4$/Fe_3O_4 showed the greatest heat capacity. The non-toxicity of this ferrifluid in solutions up to concentrations of 0.01 µg/mL against the HeLa cells was confirmed. Independently of the synthesis method, for the nanoparticles of gallium content $x > 0.8$, the superparamagnetic contribution becomes the dominant one.

Acknowledgements
This work was supported by the National Science Centre under grant OPUS no 2018/31/B/ST3/00279, the Polish Government Plenipotentiary for JINR in Dubna (Project no PWB/168-10/2021) and the Polish Ministry of Science and Higher Education under subsidy for maintaining the research potential of the Faculty of Physics, University of Bialystok.

References

[1] A. Kumar et al., Nanomedicine 6, 64 (2010)
[2] Y.M. Wang et al., J. Magn. Magn. Mat. 323, 23; 2953 (2011)
[3] P. Cherukuri et al., Advanced Drug Delivery Reviews 62, 339 (2010)
[4] E. Day et al., Journal of Biomechanical Engineering 131, 074001-1 (2009)
[5] K. Yamada et al., International Journal of Hyperthermia 26, 465 (2010)
[6] B.F. Bogacz et al., A. Phys. Pol. A. 134 (5), 993 (2018)
[7] K. Rećko, et al., Phase Transitions 91(2), 128 (2018)
[8] K. Rećko, et al., J. Surf. Investig.: x-ray synchrotron neutron tech. 14, S85–S92 (2020)

STRUCTURE OF MAGNETIC NANOPARTICLES IN BULK AND AT INTERFACES BY NEUTRON SCATTERING

Viktor I. Petrenko

BCMaterials, Basque Centre for Materials, Applications and Nanostructures, Leioa, Spain;
IKERBASQUE, Basque Foundation for Science, Bilbao, Spain
viktor.petrenko@bcmaterials.net

Results of neutron reflectometry (NR) and small-angle neutron scattering (SANS) for nanoscale characterization of magnetic nanoparticles in bulk and at interfaces will be shown. The structural analysis of various types of magnetic fluids (MFs) will be described in details during the presentation. Additionally the interaction characteristics between surfactant/polymer molecules used in stabilization of MFs were investigated, which is very important for understanding the synthesis procedure of highly stable magnetic fluids with controllable properties. The adsorption of surfactant coated magnetic nanoparticles from highly stable magnetic fluids on crystalline silicon was studied by NR. Two types of MFs based on nanomagnetite (co-precipitation reaction) dispersed and stabilized in a non-polar organic solvent (coating by oleic acid) and a strongly polar solvent (coating by sodium oleate and also modified by poly(ethylene glycol)) will be considered. It was obtained that along with the structural stability in bulk the considered MFs are characterized by the interface stability as well. No any adsorption of nanoparticles was detected from reflectometry experiments in the case of large and developed fractal in the ferrofluid with PEG addition. Also effect of external magnetic and electric fields on the behavior of MNPs will be discussed according to neutron data.

Motion of a Membrane Enzyme as Seen by SANS

W. Javed[1,2,3], C. Ebel[1], C. Orelle[2], J.M. Jault[2], A. Martel[3]

[1]*IBS; Univ. Grenoble Alpes, CNRS, CEA; Grenoble, 38000; France*
[2]*Molecular Microbiology & Structural Biochemistry (MMSB) UMR 5086; CNRS/University of Lyon; Lyon, 69000; France*
[3]*InstitutMax Von Laue Paul Langevin (ILL); Grenoble, 38000*

presenting author's email: martela@ill.fr

Small Angle Neutron Scattering is a low-resolution technique enabling to probe the solution structure of individual biomacromolecules possibly in complex with its partners. In particular, concerning membrane proteins, the membrane-like environment can be made invisible in order to see only the protein. Here, we combined SANS with X-ray crystallography, cryoEM, H/D exchange coupled with mass spectrometry and limited proteolysis to reveal the flexibility and ligand-induced conformational changes of the multidrug ABC transporter BmrA.

Limited proteolysis revealed an important flexibility of BmrA WT in most steps of its catalytic cycle. Cryo-EM provided high-resolution of the closed conformation by analysis of an artificially monodisperse sample, and X-ray crystallography data enabled to build homology models of other conformations, which constituted the starting point of SANS analysis. H/D X-MS pinpointed the flexible part along the transporter sequence and SANS revealed the extent of this flexibility.

Together, these techniques enable us to describe the ABC transporter cycle in term of successive conformational equilibria, a much more realistic and accurate vision of this biological process [1].

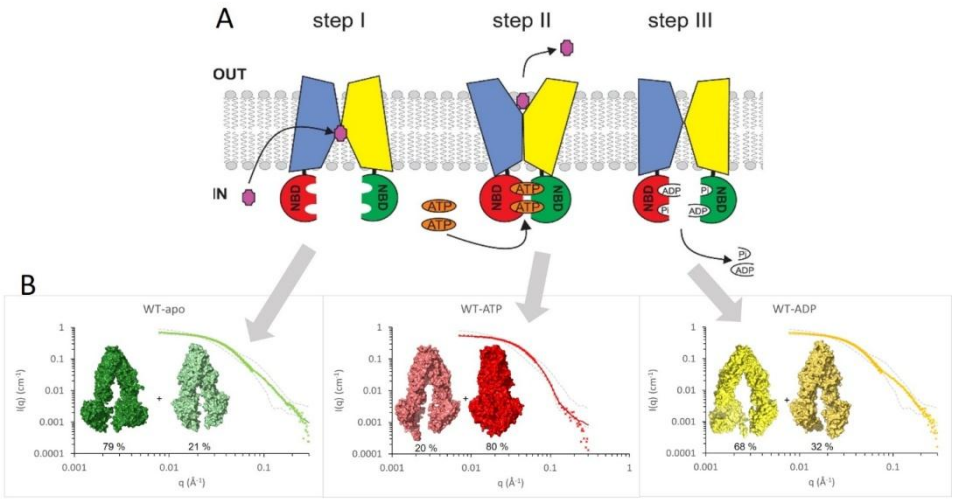

Figure 1. A: Main steps of the enzymatic cycle of ABC transporters (from [2]); B: Structural definition of these steps in solution by sequential conformational equilibria [1].

[1] Javed et al. in preparation (or submitted)
[2] Wannes Dermauw, Thomas Van Leeuwen, The ABC gene family in arthropods: Comparative genomics and role in insecticide transport and resistance, Insect Biochemistry and Molecular Biology, Volume 45, 2014

Keywords: Small Angle Neutron Scattering; Solution structure and dynamics; membrane protein; biological complexes

High-pressure effect on crystal and magnetic structure of complex nanostructured oxides of manganese and iron

N.M. Belozerova[1], S.E. Kichanov[1], E.V. Lukin[1], D.P. Kozlenko[1], Z. Jirak[2], B.N. Savenko[1]

[1]*FLNP, Joint Institute for Nuclear Research, Dubna, Russia*
[2]*Institute of Physics, 162 00 Praha 6, Czech Republic*

e-mail: nmbelozerova@jinr.ru

The study of manganites and ferrites is of great importance due to the wide variety of their structural and magnetic properties, which are interesting from the point of view of fundamental and applied research. Significant saturation magnetization, relatively high electrical resistance, low electrical losses, and good chemical stability make these compounds important for a wide range of technological applications. Complex oxides of manganese and iron are widely used in the manufacture of magnetic media for storing information, supersensitive magnetic field and temperature sensors, transformer cores, rod antennas. Moreover, such materials can be useful in biomedicine: as an effective heating agent for the treatment of cancerous tissues by means of magnetic hyperthermia, as biomarkers for MRI diagnostics and in magnetic drug delivery systems.

A wide range of magnetic properties of manganites and ferrites depends on the crystal structure of the compounds, on the particle size and external conditions (temperature, pressure). It is possible to control the properties of the synthesized compounds, by the variation of these parameters. The knowledge of relationship between magnetic and crystal structure of such compounds, which can be obtained from high-pressure investigations, is very essential for understanding the nature and mechanism of physical phenomena observed in it.

In this work, manganites$La_{1-x}Sr_xMnO_3$ (x = 0.28, 0.37, 0.47) and ferrites with the spinel structure $Zn_{0.34}Fe_{2.53}O_4$ and $Zn_{0.3}Cu_{0.7}Fe_{1.5}Ga_{0.5}O_4$ were chosen for neutron diffraction studies at high pressure and in a wide temperature range. Neutron powder diffraction measurements at ambient and high pressures up to 5.5GPa were performed on DN-6 and DN-12 diffractometers at the IBR-2 high-flux pulsed reactor [FLNP, JINR, Dubna, Russia] using the sapphire anvil high-pressure cell.

It was found that the magnetic structure of nanostructured manganites $La_{1-x}Sr_xMnO_3$(x = 0.28, 0.37, 0.47)at normal pressure and low temperatures is a superposition of two phases: a ferromagnetic and antiferromagnetic A-type phase. The observed effect of magnetic phase separation in in these compounds at normal and high pressures is described using the core-shell model. A significant change in the volume ratio of the fractions of the ferromagnetic and

antiferromagnetic phases towards the suppression of the ferromagnetic component under high pressure was found.

A significant instability of the ferrimagnetic structure of ferrite $Zn_{0.3}Cu_{0.7}Fe_{1.5}Ga_{0.5}O_4$ under high pressure was found. The behavior of the magnetic moments of iron ions in the crystallographic positions A and B in $Zn_{0.34}Fe_{2.53}O_4$ and $Zn_{0.3}Cu_{0.7}Fe_{1.5}Ga_{0.5}O_4$ferrites with changes in temperature and pressure have been studied. The lattice parameters, the lengths and angles of interatomic bonds, and the magnetic moments of iron are calculated as functions of temperature and pressure. The structural mechanisms of the magnetic transition in ferrites with a spinel structure are discussed.

The work was supported by the RFBR grant№ 20-02-00550-a.

Reversible control of magnetism in FeRh thin films

Dániel G. Merkel[1,2], Attila Lengyel[1], *Dénes L. Nagy*[1], Attila Németh[1], Zsolt E. Horváth[2], Csilla Bogdán[1], Maria A. Gracheva[3], Gergő Hegedűs[1], Szilárd Sajti[1], György Z. Radnóczi[2], Edit Szilágyi[1]

[1] *Wigner Research Centre for Physics, P.O.B. 49, 1525 Budapest, Hungary*
[2] *Centre for Energy Research, P.O.B. 49, 1525 Budapest, Hungary*
[3] *Institute of Chemistry, Eötvös Loránd University, Pázmány Péter sétány 1/A,1117 Budapest, Hungary*

email: nagy.denes@wigner.hu

Besides the traditional "faster–smaller–cheaper" directive, a new requirement has recently arisen for the newly developed devices: the energy efficiency. Therefore, the study of novel materials and developing new operation principles for energy-saving applications in information technology are essential for supporting sustainable development. From this point of view, the fine control of magnetism is a great step towards reducing energy consumption of information storage by orders of magnitude.

The nearly equiatomic Fe-Rh alloy of B2 (α, prototype: CsCl) crystal structure is an excellent playground for developing energy-efficient magnetic devices. The key phenomenon for applications is the metamagnetic transition from the low-temperature antiferromagnetic (AFM) α'' to the high-temperature ferromagnetic (FM) α' phase close to room temperature accompanied with a reduction of the resistivity and an ~ 0.6% isotropic strain of the crystal lattice. To laterally nanopattern FeRh thin films for anticipated devices, magnetic B2 regions should be separated from each other by paramagnetic (PM) A1 (γ, prototype: Cu) structured areas. Here we present a study [1] performed by conversion-electron Mössbauer spectroscopy (CEMS), high-angle X-ray diffraction (XRD), neutron reflectometry (NR), Rutherford backscattering spectrometry (RBS) and transmission electron microscopy (TEM) on an FeRh thin film deposited on MgO(100) substrate at 200 °C.

We find that the main component of the as-deposited film of $[^{nat}Fe_{51}Rh_{49}(63\ Å)/^{57}Fe_{51.04}Rh_{48.96}(46\ Å)]_{10}$/MgO(100) structure is the PM A1 phase that is fully converted to the magnetic B2 phase by annealing at 300 °C for 60 min. Subsequent irradiation by 120 keV Ne^+ ions turns the thin film completely to the PM A1 phase. Repeated annealing at 300 °C for 60 min results in 100% magnetic B2 phase, i.e. a process that appears to be reversible at least twice. The A1 → B2 transformation takes place without any plane-perpendicular diffusion while Ne^+ irradiation results in significant interlayer mixing.

As an outlook, preliminary studies [2] performed by CEMS, magnetic force microscopy (MFM), grazing-incidence nuclear resonance scattering of synchrotron radiation (NRS), RBS and field emission scanning electron microscopy (FESEM) of films covered by polystyrene and silica irradiation masks, consisting of nominally 500 nm and 1000 nm diameter spheres applied on the surface by using Langmuir–Blodgett technique are presented. The results show the feasibility of masked nanopatterning of FeRh thin films.

References

1) Merkel, D.G., Lengyel, A., Nagy, D.L. *et al.* Reversible control of magnetism in FeRh thin films. *Sci Rep* **10,** 13923 (2020). https://doi.org/10.1038/s41598-020-70899-x.

2) Merkel, D.G., Hegedűs, G., Gracheva, M. *et al.* A three-dimensional analysis of magnetic nanopattern formation in FeRh thin films. *To be published.*

Hemocyanin from the great pond snail *Lymnaea stagnalis* – protein with unique structure and anticancer activity

Kamil Szpotkowski

Institute of Bioorganic Chemistry Polish Academy of Sciences, Noskowskiego 12/14, 61-704 Poznań

The great pond snail *Lymneae stagnalis* is a widespread water snail, one of the biggest water snail in Europe. It is very often used in different laboratory tests for studying developmental biology, study of learning, memory and neurobiology [1], its embryos have been used in toxicity tests (pesticides, etc.). The growing interest in hemocyanins is due to numerous signals about their anticancer, antiviral and antibacterial properties [2].

Hemocyanin represent a big class of glycosylated proteins responsible for transporting oxygen in the hemolymph of molluscs and arthropods. Although many authors suggest that the hemocyanin plays a very important role in the snail's interactions with the environment, not much information is available about the protein.

The aim of this study was to determine the association-dissociation behavior and stability of native hemocyjanins isolated from the great pond snail *Lymneae stagnalis*. It was confirmed, that the basic quternary structure is a cylindrical decamer with a diameter of about 3.5 nm. It was also observed that easily dissociate into functional subunits at an alcalic pH and then recombine at a neutral pH. Using structural studies, allosteric mechanizm of oxygen binding was confirmed. Under normal circumastances, hemocyanin is in charge to transport oxygen, but after infection, it can transform itself into phenoloxidase to fint microbes. We confirmed, that phospohlipid addition causes structural transformation into phenolo-oxidase. Circular dichroizm was used to analyse secondary structure of hemocyanin and thermal stability. It was confirmed that hemocyanin is stabile in the temperature range 0-70ºC. *In vitro* studies of antitumour activities of hemocyanin were performed with human colon cell line HCT 116. The obtained results showed that the human colon cell line is sensitive to the action of the tested hemocyanins.

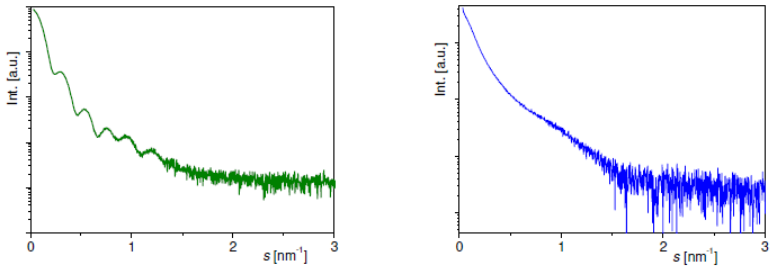

FIGURE 1. Experimental SAXS curves of hemocyanin from the great pond snail in two different conditions, at pH 8.5 (left) and at pH 10.5 (right).

Acknowledgements

The research was financed by the Plenipotentiary Representative of the Government of the Republic of Poland at ZIBJ in Dubna as part of the Cooperation Project PWB/168-24/2021

References

[1] Feng Z-P., et all. (2009) "Transcriptome analysis of the central nervous system of the mollusc *Lymnaea stagnalis*". *BMC Genomics* **10**: 451

[2] Gesheva V, et all. (2014) Anti-cancer properties of gastropodan hemocyanins in murine model of colon carcinoma *BMC Immunol.* **15**: 34.

Formation of micelle-polymer complexes in the bulk of surfactant solution and interface of polymer brush system

O.P. Artykulnyi[1,2], M.M. Avdeev[1,3], V.I. Petrenko[1], O.I. Ivankov[1], L.A. Bulavin[2]

[1]*Joint Institute for Nuclear Research, Dubna, Moscow Region, Russian Federation*
[2]*Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
[3]*Lomonosov State University of Moscow, Moscow, Russian Federation*
[4]*BCMaterials, Basque Centre for Materials, Applications and Nanostructures, 48940, Leiona, Spain*
[5]*Ikerbasque, Basque Foundation of Science, 48809, Bilbao, Spain*

E-mail: artykulnyi@jinr.ru

The unique behavior of surfactant-polymer interaction driven byself-assembly phenomena gives great variability of possible structures and plentiful phase diagrams that allows manipulating with surfaces and interfaces of nano-scale colloidal systems [1]. In this way, the magnetic nanoparticles initially stabilized by a double layer of anionic surfactant such as sodium oleate (SO), dodecylbenzene sulfonate acid (DBSA), can be modified by physicochemical adsorption of poly(ethylene glycol) (PEG) polymer chain to create a protein-resistive shell that significantly increases the average circulation time of particles in the bloodstream.

The complexation phenomena of anionic surfactant with neutral polymer PEG were studied in the bulk of solution by small-angle neutron scattering (SANS) and at the surface of polymer brush system by neutron reflectometry. The structure of surfactant-polymer complexes was obtained for a wide range of polymer molecular masses by the least-square approximation of SANS data using the model scattering intensity(Fig.1 a) [2].The effect of surfactant-polymer complex formation was obtained in the dense surrounding of PEG polymer brush the flat silicon substrate [3].

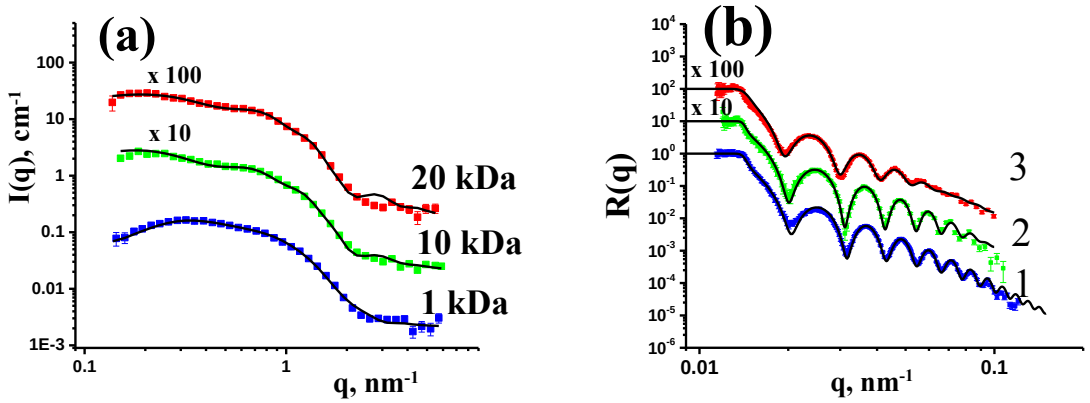

Fig. 1 Experimental SANS curves from mixed DBSA – PEG solutions with constant concentrations of DBSA (0.2 vol. %) and PEG (0.04 vol. %) and various molecular masses of PEG (a); Neutron reflectivity from PEG polymer brushes: (1) substrate, (2) PEG brush, (3) PEG brush in DBSA micellar solution (b)

[1] B. Kronberg, K. Holmberg, B. Lindman, Surface Chemistry of Surfactants and Polymers, Wiley, 2014.
[2] O.P. Artykulnyi, A.V. Shibaev, M.M. Avdeev, et al. J. Mol. Liq. (2020), 308, 113045
[3] O.P. Artykulnyi, M.M. Avdeev, Ye.M. Kosiachkin, et al. Nucl. Phys. At. Energy.(2021), 22, 149 – 156.