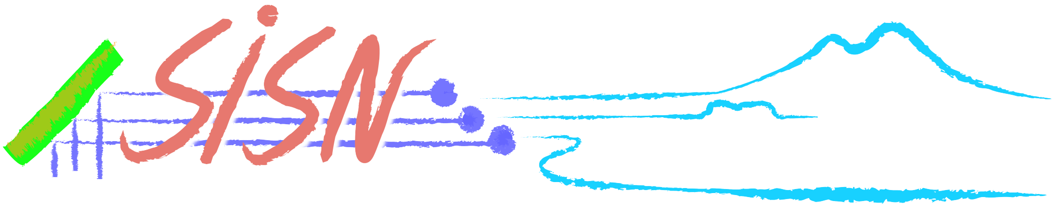

Società Italiana di Spettroscopia Neutronica

XXV Congresso Annuale

Napoli, 3-4 Luglio 2014

BOOK OF ABSTRACTS

Indice

Presentazione

Il XXV Congresso Annuale della Società Italiana di Spettroscopia Neutronica vuole essere il momento d'incontro della comunità italiana che usa i neutroni come strumento di indagine nei più diversi settori scientifici, dalla fisica alla geologia, dalla chimica alla biologia, dalla conservazione dei beni culturali fino alle discipline ingegneristiche.

Il Congresso è per sua natura aperto e interdisciplinare, con ampi spazi per la discussione dove confrontarsi, raccogliere idee e far nascere nuove collaborazioni. Tra le comunicazioni scientifche, una sessione sarà dedicata ai giovani soci SISN, studenti e dottorandi, che potranno presentare i loro primi risultati, mentre una sessione presenterà lo stato e il futuro dell'impegno europeo nella ricerca con i neutroni.

Per i soci SISN, il Congresso è completato dal momento istituzionale dall'Assemblea della Società.

Il XXV Congresso Annuale SISN si svolgerà nel cuore di Napoli, nella prestigiosa sede della Società Nazionale di Scienze, Lettere e Arti in Napoli, ospite dell'Accademia di Scienze Fisiche e Matematiche.

Parte I

Programma

Giovedì 3 Luglio

8.30 - 9.00

WELCOME & REGISTRATION

9.00 - 10.45

I SCIENTIFIC HIGHLIGHT SESSION

Chair: Luigi Paduano

Exploring the molecular mechanisms of metal-based pharmacological agents via X-ray crystallography
Antonello Merlino

Neutron reflectometry probes density profiles of proteins adsorbed onto polymer brushes
Giovanna Fragneto

Liquids and glasses structures: in situ container-less neutrons scattering experiments combining with atomistic models
Viviana Cristiglio

The Frascati Neutron Generator and 3 He-free triple GEM thermal neutron detector
Antonino Pietropaolo

10.45 - 11.10

COFFEE BREAK

11.10 - 12.40

II SCIENTIFIC HIGHLIGHT SESSION

Chair: Tatiana Guidi

New Sorgentina Fusion Source (NSFS) Experimental Facility: Supporting Materials Research
Patrizio Console Camprini

Clip talks

Solvent Extraction: Liquid-Liquid Interfaces by x-Ray and Neutron Reflectivity
Ernesto Scoppola

Nanocomposites composed of HEUR Polymer and Magnetite nanoparticles: Structure and magnetic response of the hydrogel and dried state
Antonella Campanella

The Self-assembly and polymorphism of 5′-guanosine monophosphate in the presence of excess ions
Silvia Moscatelli

Structural Characterization of Iron Oxide Based Nanoparticles: Why Core is more promising than Core-shell
Alessandra Luchini

Hsp60 can modify amyloid β peptide aggregation: a preliminary study
Caterina Ricci

12.40 - 14.30

LUNCH

14.30 - 16.15

LE INFRASTRUTTURE PER LA NEUTRONICA IN EUROPA: STATO E PROSPETTIVE

Chair: Paolo Mariani

The ESS project: status and perspectives
Caterina Petrillo

Present status and near-future perspectives of Italian neutron research at ILL
Ubaldo Bafile

The Italian activity at the ISIS pulsed neutron source
Antonella Scherillo

The IRIDE neutron source
Riccardo Faccini

BER II Neutron Facility at HZB
Thomas Gutberlet

Heinz Maier-Leibnitz Zentrum
Flavio Carsughi

16.15 - 17.15

SCIENTIFIC COFFEE: COFFEE BREAK & POSTER SESSION

17.15 - 19.00

ASSEMBLEA DELLA SOCIETÀ ITALIANA DI SPETTROSCOPIA NEUTRONICA

20.00

SOCIAL DINNER

Venerdì 4 Luglio

9.00 - 10.45

III Scientific highlight session

Chair: Piero Baglioni

Exploring the molecular mechanisms of metal-based pharmacological agents via X-ray crystallography
Frank Gabel

Structural investigation on liposomes containing Hopanoid-Lipid A: a new component of bacterial outer membranes
Giuseppe Vitiello

Functional nanostructure of the Pseudomonas aeruginosa OprF protein incorporated into a tethered lipid bilayer membrane
Marco Maccarini

L.E.N.A. - Laboratory of Applied Nuclear Energy of the University of Pavia - Neutron Facilities and Main Activities
Michele Prata

10.30 - 11.00

Coffee Break

11.00 - 12.30

IV Scientific highlight session

Chair: Renato Magli

Natural quasicrystals: Messengers from outer space
Luca Bindi

New insights into the low temperature oxygen mobility mechanism in perovskite related materials
Andrea Piovano

Morphology of mesoporous bicontinuous emulsions as probed by rheo-optical analysis and SANS
Valentina Preziosi

DREAM: Diffraction Resolved by Energy and Angle Measurements: A bispectral powder diffractometer for the future ESS source
Nicolò Violini

12.45

Conclusioni e saluti

Parte II

Invited talks

NATURAL QUASICRYSTALS: MESSENGERS FROM OUTER SPACE

L. Bindi

Dipartimento di Scienze della Terra, Università di Firenze, Firenze, Italy

The well ordered world of solid materials was forced to reassess its rules when quasicrystals were first discovered in the laboratory. Quasicrystals are solids whose diffraction patterns are composed of Bragg peaks, like periodic crystals, but with symmetries forbidden to crystals (such as five-fold symmetry in the plane or icosahedral symmetry in three dimensions). Over the last twenty-five years, more than one hundred examples have been identified, but, until now, all have been produced in the laboratory under controlled conditions ranging from rapid to moderately slow. The original theory suggested that quasicrystals can be as robust and stable as crystals, perhaps even forming under natural conditions. This thought motivated a decade-long search for a natural quasicrystal, culminating in the discovery of icosahedrite ($Al_{63}Cu_{24}Fe_{13}$), an icosahedral quasicrystal found in a museum sample consisting of several typical rock-forming minerals combined with exotic rare metal alloy minerals, like khatyrkite and cupalite, later demonstrated to be extraterrestrial in origin. The discovery of icosahedrite pushes the age of the oldest known example of this phase and quasicrystals generally back to ca. 4.5 Gy, the age of all known unequilibrated chondrites. The occurrence inside the meteorite demonstrates that quasicrystals can form naturally within a complex, inhomogeneous medium. This sample formed under astrophysical conditions; whether a quasicrystal of some type can form in the course of planetary evolution or under terrestrial conditions remains an open question, but the likely answer is 'yes', now that a first example has been found. The story demonstrates that mineralogy continues to make important contributions to science. Many new minerals have compositions and crystal structures unknown to synthetic chemistry. Perhaps we will discover further quasicrystalline materials with new compositions or new forbidden symmetries not yet observed in the laboratory, or even new phases of matter not yet conceived of.

THE BOX C/D STRUCTURE REVEALS THE MECHANISM OF RRNA METHYLATION: A STUDY COMBINING SANS, SAXS AND NMR

F. Gabel(1,2), A. Lapinaite(3), B. Simon(3), L. Skjaerven(3), M. Rakwalska-Bange(3), and T. Carlomagno(3)

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(2)*Institut Laue-Langevin, F-38042 Grenoble, France*
(3)*European Molecular Biology Laboratory, D-69117 Heidelberg, Germany*

In order to assemble fully functional ribosomes - the cell's protein factories - ribosomal RNA (rRNA) has to undergo several post-transcriptional chemical modifications. One of the most important ones is methylation of the 2'-O-ribose sugar, which is carried out by the Box C/D complex in Archea and Eukarya. Despite intensive research, the structural details and molecular mechanism of the methylation process have remained elusive for many years due to the lack of available high-resolution structures. We have solved the 390 kDa structures of the apo- and holo- Box C/D complex from *Pyrococcus furiosus* by using a powerful and innovative structural approach combining SANS, SAXS and NMR [1]. The structural study, together with an NMR-based assay that follows the methylation and release of ^{1}3C-labeled substrate RNA, allowed us to identify the sequential nature of the process, suggesting a regulatory mechanism for rRNA processing and, in fine, a potential control mechanism for ribosome assembly. Our study illustrates the power of combining SANS, SAXS and NMR to study high molecular-weight biomacromolecular assemblies. Indeed, SANS data, together with deuterium labeling and contrast variation, were crucial to determine the respective positions of the protein and RNA subunits within the apo- and holo-complexes for the NMR-modeling process. Moreover, the SANS and SAXS data allowed us to validate the overall shape and stoichiometry of the complex.

[1] A. Lapinaite et al., Nature **502**, 519-523 (2013)

EXPLORING THE MOLECULAR MECHANISMS OF METAL-BASED PHARMACOLOGICAL AGENTS VIA X-RAY CRYSTALLOGRAPHY

A. Merlino

Department of Chemical Sciences, University of Naples Federico II, Napoli, Italy

Since the introduction of Cisplatin in clinical trials for the treatment of certain cancers, antitumor metallopharmaceuticals have attracted significant attention. Cisplatin, Oxaliplatin and Carboplatin are Pt(II) complexes that are largely used for the treatment of many solid tumors. Although the exact mechanism of action of these compounds is still not fully elucidated, it appears that the cellular target of these molecules is DNA. As alternative approaches to platinum, a number of Ru(II) and Ru(III), Au(I) and Au(III) coordination compounds are considered potential anticancer agents due to their relevant antiproliferative activity. The mechanism of action of these compounds is unknown, but it is likely that it involves interactions with biomolecules other than DNA; adduct formation with proteins must be considered. The present talk will present the results of structural characterizations, carried out mainly by X-ray crystallography, of the interactions between a number of Pt(II), Ru(III), Au(III) and Au(I) compounds and proteins [1-8]. The results will be discussed in relation to the possible mechanism of action of these metallodrugs.

[1] A. Vergara et al., Inorg Chem **52**,4157-9 (2013)
[2] L. Messori et al., Inorg Chem **52**,13827-9 (2013)
[3] A. Vergara et al., Inorg Chem **52**,10714-10716 (2013)
[4] L. Messori et al., Chem Comm **49**,10100-10102 (2013)
[5] L. Messori et al., Metallomics **6**, 233 - 236 (2014)
[6] L. Messori, A. Merlino. Dalton Trans. **43**, 6128-31 (2014)
[7] L. Messori, A. Merlino. Inorg Chem **53**, 3929-31 (2014)
[8] L. Messori et al. Angew Chem Int Ed Engl. (2014), in press. doi: 10.1002/anie.201403337.

Parte III

Scientific highlights

New Sorgentina Fusion Source (NSFS) Experimental Facility Supporting Materials Research

P. Console Camprini(1), D. Bernardi(1), M. Frisoni(2), M. Pillon(3), A. Pietropaolo(3), M. Angelone(3)

Associazione ENEA-EURATOM Sulla Fusione, ENEA
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(2)*ENEA Centro di Ricerca di Bologna, 40129 Bologna, Italy*
(3)*ENEA Centro di Ricerca di Frascati, 00044 Frascati , Rome, Italy*

Within the framework of research and development on fusion technology, a 14 MeV neutron source has long been considered as a key facility to perform irradiation tests supporting design and licensing of DEMO reactor. In this context, New Sorgentina Fusion Source (NSFS) project has been proposed taking advantage of well-established D-T generators technology, properly scaled in order to design a bright neutron source of some $10^1$5 n/sec. It is based on multiple 200 keV deuterium and tritium ion beams, produced and accelerated by means of ion generators and extraction grid proven technology currently utilized in neutral injectors at large experimental tokamaks. Beams deliver several Amperes towards a deuterium-tritium enriched layer on a rotating target where fusion reactions take place. Tests on materials damage upon neutron irradiation are intended to be performed with the actual 14 MeV neutron spectrum typical of fusion reactors. NSFS project is intended to be carried out within national as well as international collaborations in order to provide a fusion-related neutron source but also a multipurpose facility. In present contribution, the main facility characteristics are highlighted along with expected irradiation performances.

LIQUIDS AND GLASSES STRUCTURES: IN SITU CONTAINER-LESS NEUTRONS SCATTERING EXPERIMENTS COMBINING WITH ATOMISTIC MODELS

V. Cristiglio

Institut Laue Langevin, Grenoble (France)

The sample environment is a critical component of research programs in advanced materials, geological systems, biology, and energy-related applications.

Over the past ten years an increasing number of studies on liquid materials have been carried out thanks to the container-free sample handling methods. Techniques based on aerodynamics levitation have created new opportunities for investigating the structure of high-temperature liquids (up to 3000 K) and during their glass transition with a very high degree of temperature and chemical composition control. Several installations of the aerodynamics levitation have been developed at ILL to allow studies on molten materials.

A new method recently in development at ILL is based on acoustic levitation. The technique was originally designed to study the evaporation rate of pure solvent droplets suspended in a dry in gas, but was later extended to studies of solution droplets. Evaporation of the solvent during levitation gradually decreases the volume of the droplet and therefore increases the corresponding concentration of the solute. This allows to study phenomena like aggregation and crystallization in situ and to quickly find suitable crystallizing conditions.

In this talk these container-less techniques will be presented and some related results of structure investigation made by neutrons scattering will be discussed. The experimental data will be compared with molecular dynamics calculation models always developed at ILL.

A second part of this talk will be dedicated to present the D16 cold-neutron diffractometer at ILL. The major characteristics, performances and new directions of the D16 instrument will be exposed.

Neutron reflectometry probes density profiles of proteins adsorbed onto polymer brushes

E. Schneck(1,2), A. Schollier(1,3), I. Berts(1,4), A. Halperin(5), M. Sferrazza(3), G. Fragneto(1)

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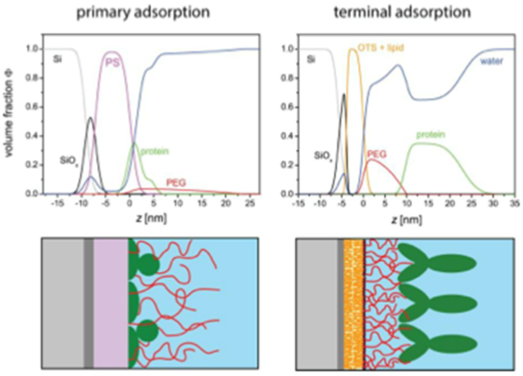
(2) *Max Planck Institute of Colloids and Interfaces, Potsdam, Germany*
(3) *Université Libre de Bruxelles, Brussels, Belgium*
(4) *Ludwig-Maximilians-Universität München, Germany*
(5) *Université Joseph Fourier Grenoble, Saint-Martin d'Hères, France*

The density profiles of proteins adsorbed onto poly(ethylene glycol) (PEG) brushes are characterized by neutron reflectometry (NR). In contrast to conventional methods, NR allows directly distinguishing among primary adsorption at the grafting surface, secondary adsorption at the brush outer edge, and ternary adsorption to the polymer chains [1]. For hydrophobic grafting surfaces, myoglobin (Mb) exhibits primary adsorption, which consists of two distinct protein layers. The amount of Mb adsorbed in the inner layer is independent of the polymerization degree N but varies with the grafting density σ, while for the outer layer it is correlated to the amount of grafted PEG and thus depends on both N and σ. The sensitivity of NR is enhanced by the use of deuterated Mb [1]. PEG antibodies, whose implications in the field of biocompatible functionalization are still underexplored, exhibit terminal binding to the chain end groups and form dense layers covering the brush periphery. Precise structural studies by NR provide a valuable basis for the rational design of protein-repellent surface functionalization and may help understand the mechanisms by which antibodies lead to brush failure in in-vivo applications.



[1] E. Schneck, A. Schollier, et al. Langmuir **29**, 14178 (2013)

FUNCTIONAL NANOSTRUCTURE OF THE *Pseudomonas aeruginosa* OprF PROTEIN INCORPORATED INTO A TETHERED LIPID BILAYER MEMBRANE

M. Maccarini(1), L. Gayet(1), B. Stidder(1), J.-P. Alcaraz(1), E. Watkins(2),
J.-L. Lenormand(1), and D. Martin(1)

(1) *TIMC/IMAG, Grenoble, France*
(2) *Institut Laue Langevin, Grenoble, France*

Infection by the bacterium *Pseudomonas aeruginosa* is a serious problem for patients who are hospitalized with cancer, cystic fibrosis and burns. The case fatality rate in these patients is near 50%. *P. aeruginosa* is primarily a nosocomial pathogen and the fourth most commonly-isolated nosocomial pathogen accounting for 10% of all hospital-acquired infections. It causes urinary tract infections, respiratory system infections, dermatitis, soft tissue infections, bacteremia, bone and joint infections, gastrointestinal infections and a variety of systemic infections, particularly in patients with severe burns and in cancer and AIDS patients who are immunosuppressed.

Strains of the *P. aeruginosa* bacterium are resistant to most of the common antibiotics used in hospitals, due mainly to the low permeability of its outer membrane. We are using neutron scattering (NS) to investigate the nanoscale structure of one of the main proteins responsible for the permeability of the outer membrane of the *P. aeruginosa* bacterium, OprF. NS allows us to probe the biological function of the membrane protein in its functional state. These investigations are not possible using the classical techniques of biology.

OprF is a very novel target for new drugs that will kill bacteria resistant to standard antibiotics, such as *P. aeruginosa*. In our laboratories a novel cell-free method to synthesis the protein has been developed. By means of advanced biochemical techniques we are able to include it in model biological membranes that are grafted to gold electrodes. To provide insight into the nanoscale structure of OprF-lipid systems, we used neutron reflectometry (NR). NR allowed us to characterize the structural details of the lipids, the amount of the protein embedded in the lipid bilayer, and the orientation of the portion of the protein which extends from the membrane with unprecedented resolution. This study showed that OprF purified using the cell free protocol and incorporated into tethered lipid bilayer provides a controllable (and measurable at the nanoscale) biomimetic system constructed in vitro. This system provides the means to identify ways to control membrane proteins, and hence to open possibilities of finding new drugs that are not antibiotics, which could help to fight the serious infections caused by *P. aeruginosa*.

THE FRASCATI NEUTRON GENERATOR

A. Pietropaolo, F. Andreoli, M. Angelone, S. Loreti, G. Pagano, M. Pillon

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The Frascati Neutron Generator (FNG) is neutron source designed and realized at the Neutron Generator Laboratory of the ENEA Frascati Research Centre. The laboratory operates in the research and development framework of EFDA program for Magnetic Confinement Controlled Thermonuclear Fusion.

FNG produces almost monochromatic neutron with 2.5 MeV and 14 MeV energies exploiting fusion reactions using accelerated deuterons (up to 300 keV energy) impinging onto deuterium or tritium containing solid targets, respectively.

Intense yields can be achieved as high as 10^9 n/s for 2.5 MeV and 10^11 n/s for the 14 MeV. These yields, that can be tuned by modifying the deuteron current, allow different kind of irradiations to be performed:

- Cross sections measurements and neutron transport database validation through Benchmark and Mock-up irradiations for fusion neutronics study.
- Neutron induced materials activation.
- Calibration and characterization of fast neutron detectors.
- Single Event Effects in electronics.
- Neutron irradiation of biological samples.

Together with the neutron source the laboratory is equipped with calibrated High-Purity Germanium detectors (40% and 60% relative efficiencies) and a $\beta - \gamma$ coincidence detector.

An upgrade is foreseen to setup a thermal neutron irradiation station characterized by a high homogeneity over a surface of 50×50 cm^2 and an optimized Cd ratio to provide almost Maxwellian neutron spectrum. This facility, where both thermal neutrons and fast neutron can be available, will be exploited, for neutron detector characterization for different applications like He-replacement activity, homeland security, characterization of neutron instrumentation and components.

In this talk the main characteristics of FNG will be outlined, the research activity presented and future perspectives for the neutron users and developers community discussed.

^{3}He-free triple GEM thermal neutron detector

A. Pietropaolo(1), G. Claps(1), F. Murtas(2), G. Celentano(1), A. Santoni(1), A. Vannozzi(1), L. Quintieri(3)

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(3)*ENEA Casaccia Research Centre, Via Anguillarese 301, 00123 S. Maria di Galeria (Rome), Italy*

A novel type of thermal neutron detector based on the gas electron multiplier (GEM) technology is presented in the framework of the research and development activity on the ^{3}He replacement for neutron detection. The device relies on a series of boron-coated alumina sheets placed perpendicularly to the incident neutron beam direction. A first prototype of the device mounting only four sheets was developed at INFN-Frascati and tested at the TRIGA reactor (ENEA-Casaccia) to assess its performances in terms of efficiency and dynamic range, being also corroborated by Monte Carlo simulations.

A new prototype version was tested on beam at the High Flux Isotope Reactor at the Oak Ridge National Laboratory (US) to assess its performance in terms of beam position resolution, efficiency and signal-to-background (S/B) ratio as compared to a 10 bar ^{3}He tube for sub-thermal neutrons. The obtained results, that are going to be presented in this contribution, demonstrate the effectiveness of the proposed detector configuration to achieve a good spatial resolution and, in the perspective, a higher thermal neutron efficiency, comparable to ^{3}He tubes typically used for diagnostic in nuclear reactors. Furthermore, the main issues to be addressed to reach the goal, mostly related to boron coating procedures and characterization, will be also pointed out.

NEW INSIGHTS INTO THE LOW TEMPERATURE OXYGEN MOBILITY MECHANISM IN PEROVSKITE RELATED MATERIALS

A. Piovano(1), A. Perrichon(2), S. Corallini(2), G. Agostini(3), M. Ceretti(2), M. Zbiri(1),
M. Johnson(1), C. Lamberti(3), and W. Paulus(2)

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(3)*University of Torino, Department of Chemistry, Torino, Italy*

Oxygen ion conductors at low temperatures are materials of major interest for a series of applications as fuel cells, battery electrodes and sensors. For this reason the discovering of oxygen reversible intercalation into brownmillerite-type $SrMO_2 \cdot 5$ (M = Co, Fe) in an electrolyte at RT has been considered of paramount importance [1-3]. By means of different inelastic scattering experiments and DFT calculations we had found evidence of the existence of a low energy mode related to a modification of oxygen dynamics in these compounds.. Nevertheless to generalize the mechanism to the whole class of perovskite related materials similar experiments should be performed on other systems. Only finding similarities on their dynamical behavior it is possible to generalize the model of phonon assisted mobility in low temperature oxygen conductors. Here we present, together with well established results on iron based brownmillerites, interesting experimental findings on a purely ionic conductor brownmillerite Sr_2ScGaO_5 and a mixed conductor with fluorite structure $NdNiO_4^+d$. Combination with DFT and MD calculations allowed highlighting similarities and differences in the oxygen diffusion mechanism, which is however shown to be always based on a modification of a specific low energy collective vibration.

[1] A. Piovano et al., J. Phys. Chem. C., **115**, 1311 (2011).
[2] W. Paulus, et al., J. Am. Chem. Soc., **130**, 16080 (2008).
[3] R. Le Toquin, et al., J. Am. Chem. Soc., **128**, 13161 (2006).

L.E.N.A. - LABORATORY OF APPLIED NUCLEAR ENERGY OF THE UNIVERSITY OF PAVIA - NEUTRON FACILITIES AND MAIN ACTIVITIES

D. Alloni(1,2), G. Bellani(1), M. Giordano(1), F. Lana(1), G. Magrotti(1,2), S. Manera(1),
F. Marchetti(1), **M. Prata**(1,2), A. Salvini(1,2), G. Vinciguerra(1)

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The TRIGA® (Training Research and Isotopes-production General Atomics) Mark II nuclear research reactor installed at the Laboratory of Applied Nuclear Energy (L.E.N.A.) of the University of Pavia is licensed for operating at 250 kW power in steady state. It was brought to its first criticality in 1965 and since then it was used for several scientific activities in different research fields. It is available for national and international collaboration in various research field. It offers different in- and out-core neutron irradiation channels, each characterized by different integral and differential neutron spectra. Neutron facilities and main activities at LENA will be described.

MORPHOLOGY OF MESOPOROUS BICONTINUOUS EMULSIONS AS PROBED BY RHEO-OPTICAL ANALYSIS AND SANS

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(2)*Dipartimento di Scienze Chimiche, Università degli Studi di Napoli, Federico II*
(3)*CSGI, Consorzio Interuniversitario per lo sviluppo di Sistemi a Grande Interfase, Florence, Italy*
(4)*CEINGE Advanced Biotechnologies, Napoli, Italy*

Microstructured mesoporous emulsions are often exploited as drug delivery systems, in particular for dermal delivery [1]. Such mesophases can be obtained by addition of water at very low addition rate into an agitated oil/surfactant solution at fixed temperature, whereby surfactants hydration may leads to sponge, lamellar, cubic or hexagonal arrangements [2], as often probed by small angle neutron scattering profiles. These bi-continuous surfactants solutions show highly viscoelastic behavior and may display also some features typical of lyotropic liquid crystalline phases. These systems show a continuous interplay between viscoelastic phase separation and surfactants self-organization, thus displaying a variety of morphologies [3]. This work has been focused on morphology characterization of the bicontinuous phases of a system composed of mineral oil, two non-ionic surfactants (one hydrophilic and one hydrophobic) and distilled water. During all the experiments, temperature was kept constant at room temperature. The phase inversion composition method, i.e., the dropwise addition of water to the oil-surfactant mixture was exploited to obtain the mesoporous bicontinuous structure. To outline bicontinuous emulsion morphology development, confocal microscopy, rheological measurements and small angle neutron scattering analysis have been exploited. Rheological measurements probed the increased viscoelasticity induced by water addition up to the point of bicontinuous phase formation. Confocal microscopy revealed the formation of complex mesoporous structures at the microscale, linked with a sponge-phase nano-structure as probed by SANS data.

[1] M. Gosenca, M. Bešter-Rogač, e M. Gašperlin, Eur. J. Pharm. Sci. , **50**, 114-122 (2013).
[2] M. Duvail et al., J. Chem. Phys. **140**, 164711 (2014).
[3] Y. Iwashita and H. Tanaka, Nature materials **5**, 147-152 (2006).

DREAM: DIFFRACTION RESOLVED BY ENERGY AND ANGLE MEASUREMENTS A BISPECTRAL POWDER DIFFRACTOMETER FOR THE FUTURE ESS SOURCE

N. Violini(1), W. Schweika(1,2), K. Lieutenant(3), A. Houben(4), P. Jacobs(4) and P.F. Henry(2)

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(2)*European Spallation Source ESS AB, Lund, Sweden.*
(3)*Helmholtz Zentrum Berlin, Germany.*
(4)*RWTH Aachen University, Germany.*

Within the ESS Design Update Program, funded by the German Federal Ministry of Education and Research, we developed the proposal of DREAM, a neutron powder diffractometer at the future European Spallation Source (ESS). Typical applications will be the determination of structures in piezo-electric and ferroelectric compounds, metal-organic frameworks, microporous polymers, complex magnetic systems, organic and inorganic hybrids and nanoparticles, multiferroics, thermoelectric materials and in-situ phase transitions in reactive or functional materials, under conditions close to operation. DREAM adopts a flexible neutron wavelength band from 0.5 Åto 4.6 Å. A 10×10 mm^2 eye-of-the-needle [1] at 6 m from the moderator enables to fit in counter rotating disc choppers that provide flexible time resolution from 10 μs to 1 ms. The best time resolution yields a d-resolution of 2.8×10^{-4} Åin back-scattering, while tuning the instrument to high intensity the flux will be sufficient to study changes on the ms timescale. Recent developments led to a new detector concept [2] based on 10 B coated cathodes, which covers 6 sr solid angle almost free of any blind areas, with a high efficiency of 50 to 70%. The 2D high spatial resolution of 4 mm will support the recognition of preferred orientation and texture and single crystal diffraction. DREAM will have 1-2 orders of magnitude more flux than world-class instruments.

[1] A. Houben et al., Nucl. Instr. Meth. Phys. Res. A **680**, 124 (2012).

[2] G. Modzel et al., Nucl. Instr. Meth. Phys. Res. A, accepted.

STRUCTURAL INVESTIGATION ON LIPOSOMES CONTAINING HOPANOID-LIPID A: A NEW COMPONENT OF BACTERIAL OUTER MEMBRANES

G. Vitiello(1,2), A. Luchini(2,3), R. Heenan(4), A. Silipo(2), A. Molinaro(2), G. D'Errico(2,3), L. Paduano(2,3)

(1)*Department of Chemical, Materials and Industrial Production Engineering, University of Naples Federico II , Naples, Italy*
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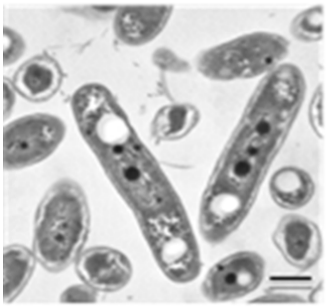
Infection Lipopolysaccharides (LPSs), major components of the outer membrane of Gram negative-bacteria, are essential for bacterial growth and survival. They act as a structural barrier and play an important role in the pathogenic or symbiotic interaction with eukaryotic hosts. We have recently demonstrated that a photosynthetic *Bradyrhizobium* strain synthesizes a novel LPS bearing a covalently attached hopanoid to the lipid A portion. Hopanoids are pentacyclic triterpenoid derivatives and constitute an important class of membrane compounds widely distributed in a diverse range of bacteria, including some rhizobia. These molecules are thought to act as membrane stabilizers, control fluidity and permeability and assure integrity of bacterial cell envelope.

In the present research, we have investigated the microstructure of liposomes, biomimicking the *Bradyrhizobium* outer membrane, which are also formed by POPE and POPG phospholipids and containing the LPS lipid A covalently substituted by a hopanoid skeleton, named BTAi1, by Small-Angle Neutron Scattering (SANS). In particular, we have obtained structural information on the thickness of the mimic Bradyrhizobium outer membrane vesicles, shedding light on the variation that may occur in vesicles morphology, membrane thickness, and size in the presence of hopanoid-bonded LPS or of its derivative. In details, we performed SANS measurements on phospholipid liposomes in the presence and absence of BTAi1, or containing a BTAi1 mutant, named BTAi1Δ*shc* (i.e. a LPS Lipid A without hopanoid moiety). The effect of $MgCl_2$ salt on the mesoscopic and microscopic properties of these aggregates was also investigated. The aim of this biophysical analysis is to correlate the structural properties of this novel lipid A specie to the complex architecture of the bacterial outer membrane, which consequently modulates the cell wall resistance.



Parte IV

Clip talks

NANOCOMPOSITES COMPOSED OF HEUR POLYMER AND MAGNETITE NANOPARTICLES: STRUCTURE AND MAGNETIC RESPONSE OF THE HYDROGEL AND DRIED STATE

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The incorporation of inorganic nanoparticles into polymer matrix has extended the particle application because of the several advantages of the polymer thin films like homogeneity and tunable physicochemical properties by increasing mechanical, magnetic and conductive properties. Such kind of nanocomposites are suitable for several modern applications, e.g. as electromagnetic wave absorbers, photovoltaic cells, OLED, data storage. In this context, the object of our study are nanocomposite systems composed by a polymer matrix which consists of hydrophobically modified ethoxylated urethane polymers (a relatively new class of industrially important macromolecules, which are gaining increasing industrial use due to their ability to impart improved rheological behavior to particulate dispersions) with core-shell magnetite nanoparticles embedded. The shell of the magnetite nanoparticles is composed by oleic acid and oleylamine, in order to provide more stability in organic solvent. We are now focusing on the structural characterization of such nanocomposites in two different morphologies: as thin dry films and as hydrogels, in order to understand the influence of the water on the structural organization of the system. The presence of magnetic nanoparticles in the dry polymer matrix shows also an interesting magnetic aspect of the system, which could be interesting for specific applications mentioned above.

STRUCTURAL CHARACTERIZATION OF IRON OXIDE BASED NANOPARTICLES: WHY CORE IS MORE PROMISING THAN CORE-SHELL

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Nowadays, Fe_3O_4 iron oxide nanoparticles have attracted attention as highly performing contrast agents for Magnetic Resonance Imaging technique (MRI), aiming to early detection of several pathologies, such as cancer. Indeed, Fe_3O_4 nanoparticles exhibit superparamagnetic properties responsible for influencing transversal proton relaxation time (T2). However, some concerns about the biocompatibility are limiting their use in the biomedical field. For this reason, nanoparticle systems combining Fe_3O_4 iron oxide with other inorganic and organic components are now very common in the literature. Here we present a complete structural characterization of Fe_3O_4-gold core-shell nanoparticles (Fe_3O_4-Au NPs), on which we implemented a novel functionalization strategy, based on the use of phospholipids, known biocompatible molecules. Fe_3O_4-Au NPs were synthesized trough the thermal decomposition method, coated with oleic acid and oleylamine, used as stabilizing agents in order to control nanoparticle size. The functionalization protocol that we introduced exploits the hydrophobic layer composed by oleic acid and oleylamine to introduce a second amphiphilic layer. In particular, we tested this functionalization strategy for several amphiphilic molecules, differing for the structure of both the nonpolar and polar portion.

Physico-chemical characterization on the prepared systems was carried out comparing the functionalized and non-functionalized Fe_3O_4-Au core-shell NPs with just Fe_3O_4 core NPs. We demonstrated that in order to fully shed light on the structure of this kind of system different photon, electrons and neutrons scattering and spectroscopic techniques have to be combined. Furthermore, the results obtained pointed toward the inability, at least for the used synthetical protocol, of producing a real Fe_3O_4-Au system without corrupting the iron oxide. Thus, according to our evidences, only the Fe3O4 core nanoparticle is promising for the biomedical application. With the present contribution, we intend to provide useful information to the researchers working in the nanoparticles field, and also to present our novel functionalization protocol for the obtainment of potentially highly biocompatible iron oxide based nanoparticles. Indeed, the functionalized nanoparticles present all the characteristics for a suitable application in detection of pathologies such as cancer, but also as nanocarries for drug delivery, being an innovative thernostic device.

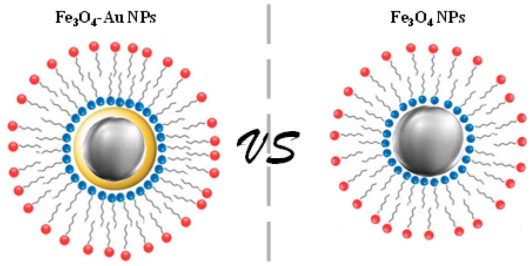

Figura 1: Schematic comparison between Fe_3O_4-Au NPs and Fe_3O_4 NPs structure. Blue head molecules represent oleic acid and oleylamine stabilizing agents, while red head molecules represent amphiphilic molecules used during functionalization.

THE SELF-ASSEMBLY AND POLYMORPHISM OF 5′-GUANOSINE MONOPHOSPHATE IN THE PRESENCE OF EXCESS IONS

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The self-assembly of biomolecules, in particular of one of the four DNA nucleotides, the 5′-guanosine monophosphate (GMP), is a current and relevant field of research. GMP is able to create in aqueous solutions and in the presence of the proper monovalent cations supramolecular structures as G-quartets, G-octamers and G-quadruplexes (which are made by the stacking of G-quartets). To understand the process of formation of these structures is very relevant, as it has been demonstrated that G-rich sequences in telomeres (the single-stranded DNA regions at the end of chromosomes) have the intrinsic capacity to fold into such non-canonical secondary structures: this folding runs to the effective capping or sequestering chromosome ends, reducing the efficiency of primer extension by telomerase. Studies about G-quartet structures have been exploited to analyse stability, self-assembling mechanism and structural properties in order to develop new strategies for novel anti-cancer agents. Moreover, G-quartets have drawn attention in nanotechnology as building blocks of molecular nanowires for nanoelectronics, as the large number of stacked quartets in G-quadruplex provides better conditions for π-overlap compared to the base-pairs of the canonical double-stranded DNA, and higher structural rigidity and stability under various conditions, increasing the probability of charge migration through the G-wires. In any case, the role of cations is very relevant and still unclear.

In this work, we present an X-ray diffraction study on the formation of GMP self-assembling structures in the presence of Ag^+ ion. As a result, it is observed that silver ions give rise to different molecular structures in respect to the other ions widely studied, such as K^+, Na^+, Li^+ and NH_4^+, that promote G-quartet based self-association. Indeed in presence of silver ions GMP forms dimeric structures. The possible biotechnological role will be discussed and to verify this preliminary observations in the near future Small Angle Neutron Scattering (SANS) studies will be executed.

HSP60 CAN MODIFY AMYLOID β PEPTIDE AGGREGATION: A PRELIMINARY STUDY

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The ultimate aim of this research project is to develop new basic knowledge about the design of an innovative therapeutic strategy for Alzheimer disease (AD). This strategy will be built considering Heat Shock Proteins (Hsp) involvement in AD. A therapeutic approach resulting from the combination of Hsp and new generation anti-aggregation compounds of increased efficiency due to in-silico design, will be conceived. The development of this innovative approach toward AD has to achieve some specific final objectives which focus to the acquisition of fundamental knowledge for the implementation of a new treatment. The description of the interaction between amyloid β peptide (Aβ) and chaperons Hsp60 and Hsp70, involved at different levels in AD, until the molecular detail, is of fundamental importance for the success of this research. Recent results demonstrated the influence of Hsp60 in Aβ peptide aggregation pattern (Thioflavin T Fluorescence spectroscopy experiments), but basic knowledge about Hsp60 activity influence toward Aβ peptide aggregation is still lacking. The first step of this research is embodied by the study of the interaction between Aβ and Hsp60, the human homolog of the bacterial GroEL. First of all, we determined that Hsp60 and GroEL present structural, energetic and stability differences. To clarify Hsp60 structure and in solution behaviour, an investigation using complementary techniques (SAXS, CD) has been performed. In particular, the interaction between Hsp60/GroEL and guanidine hydrochloride provides information on the conformational transition induced by chemical denaturation, hence on their stability. Further SAXS experiments are planned to evaluate the possible presence of a Hsp60-Aβ aggregate, hence SANS should be the concluding experiment in order to better clarify the structure of the aggregate, using the contrast variation method.

SOLVENT EXTRACTION: LIQUID-LIQUID INTERFACES BY X-RAY AND NEUTRON REFLECTIVITY

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Liquid-Liquid (LL) or solvent extraction is a separation process [1] which is based on the transfer of a solute from a solution 1 towards an immiscible phase 2, the contact with which can be enhanced by emulsification. In other terms, it is a partitioning method used to separate compounds based on their relative solubility in two different immiscible liquids, usually water and an organic solvent. The solubility is enhanced via the use of complexing molecules (an extractant) either hydrophilic or lipophilic, that are slightly amphiphilic [2,3]. The ultimate aim for application is to develop a selective transfer more cheaply and more quickly, although a trade-off always exists between selectivity and kinetics. The extraction mechanisms as well as their kinetics at molecular scale across the interface are still poorly understood even if attempts have been made [4][5]. In any case, the hydrated or solvated species (as a function of the transfer direction) have to explore various crossing configurations - very often different from those existing in bulk - associated to energy barriers that determine a part of the kinetics. Several unknown variables are left to quantify the energy barrier of the ion sorption and desorption at the active interface and in a complex association with the extractant molecules [6]. In other words, the interfacial concentration and distribution (of ions and extractants) at equilibrium but also out of equilibrium have to be determined during the ion transfer process. Since the extraction process depends both on the extractant concentration in oil and ions in water, our purpose is to measure interfacial structure changings, trying to be sensitive both at ions (Neodymium and Lithium Nitrate) and extractanct (DMDBTDMA or Diamide).For that purpose we designed a new cell both for x-Ray and Neutron reflectivity tested for experiments at ESRF (Grenoble) and J-PARC (Japan). On one side, with x-Ray, the low contrast between diamide and oil gives us access to informations about the ions-diamide interaction at interface. On the contrary, with neutron reflectivity, we can work with isotopic substitution, obtaining more informations about extractant distribution in bulk and at interface.

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Parte V

Posters

PVA NANOGELS: KINETIC AND STRUCTURAL DETERMINATION

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The aim of the present work is to prepare an innovative polymeric system for drug delivery based on polyvinyl alcohol (PVA) nanogels, able to load high drug amount and subsequently to release it over a large time period. Several synthetic polymers are reported in literature for nanogels preparation. Among them, the polyvinyl alcohol can be considered the most suitable for drug delivery applications due to its chemical and physical proprieties. PVA is a biocompatible nonionic polymer, obtained through free radical polymerization of vinyl acetate with subsequent hydrolysis of acetate groups to hydroxyl moieties. PVA is characterized by a lack of stereoregularity, and because of the presence of -OH groups in its chains, it has a strong tendency to make intra and intermolecular hydrogen bonding. Due to this PVA/water system presents a physical gelation. Here we present a small-angle neutron and microscopy investigation on such nanogels. The performed experiments revealed that PVA nanogels are water rich bicontinuous network of polymer chains. Furthermore, the formation and growth of PVA aggregates in solution has been properly investigated by dynamic light scattering (DLS) experiments. The obtained results confirmed that the aggregation process involves the growth of initial clusters, that is possible to control through addiction of salt. Indeed, studying the effects of salting-out on PVA in presence of NaCl, the prepared solution shows an increasing opalescent aspect, despite this precipitation of aggregates is not observed. In fact, the aggregates preserve their sizes and their structures are particularly water rich, so the precipitation is avoided. Moreover, salt concentration and chemical composition modulates the kinetics and the nature of the aggregation process. In conclusion, the simple preparation protocol of the system and the high biocompatibility of PVA, make these nano-structures promising carriers of molecules of biological or pharmacological interest.

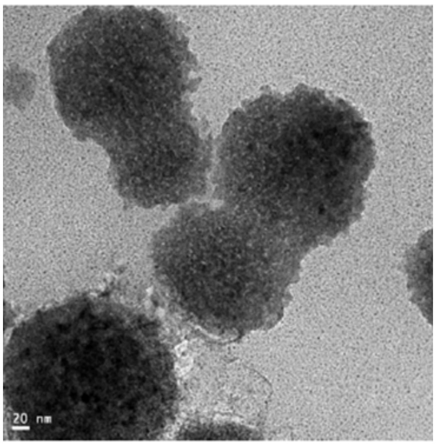

Figura 2: TEM image for PVA nanogels.

MICELLAR SYSTEMS FOR THE REMOVAL OF POLYMER COATINGS FROM WALL PAINTINGS - A STUDY ON THE NANO-STRUCTURE AND THE CLEANING MECHANISM

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Nanostructured soft matter systems represent effective and long-lasting solutions with respect to traditional and often obsolete methodologies for the conservation of works of art. In particular, complex fluids such as micelles and microemulsions are the most performing media for the removal of organic materials from porous supports, like wall paintings or stones. We report on the characterization of two systems, EAPC and XYL, which have shown excellent performances in the removal of organic polymers from wall paintings. EAPC is a five-components fluid composed of water, sodium dodecylsulfate (SDS), 1-pentanol (PeOH), propylene carbonate (PC), and ethyl acetate (EA), while XYL is a classical o/w microemulsion, where p-xylene droplets are stabilized in water by SDS and PeOH. Small-angle neutron scattering (SANS) with contrast variation is used to infer a detailed picture of the structure of these complex fluids, with a particular focus on the partition of the components between the bulk phase and the nanocompartments. We found that, differently from XYL, the EAPC system is neither a microemulsion nor a simple micellar solution, with the cosolvents partitioned between the dispersing phase and the disperse droplets. These different structural features play a key role in defining the cleaning effectiveness and specifically the kinetics of interaction between the nanofluid and the polymeric coating to be removed, which is of paramount importance for the application in the field. Both of these nanofluids are effective in polymer removal, but EAPC is considerably more efficient and versatile. The structural properties of these nanofluids and of the polymer film were investigated before, during and after the interaction process using several surface and solution techniques. Rather than a classical detergency mechanism, we demonstrated that micelles act as solvent containers and interact with the polymer film leading to its swelling and detachment from the surface and to its segregation in a liquid droplet, which phase-separates from the aqueous bulk. After the removal process the micelles become smaller in size and undergo a structural re-arrangement due to the depletion of the organic solvents. These findings can be framed in an interaction mechanism which describes the removal process, opening up new perspectives in the design and formulation of new cleaning systems specifically tailored for intervention on particular conservation issues.

A CATION-TEMPLATED FULLY-ANTI DODECAMER FORMED BY A (5'S)-5',8-CYCLO-2'-DEOXYGUANOSINE DERIVATIVE

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It is well-known that guanosine and deoxyguanosine- 5?-monophosphate (GMP and dGMP) and several of their derivatives show in water a hierarchical self-assembling process, which starting from the formation of guanosine tetramers (G-quartets) ends up at the appearance of cholesteric and hexagonal lyotropic phases. Guanine is indeed a multiple H-bonding unit, presenting both H-bond acceptor and donor groups, and in the G-quartets four guanine bases are associated through Hoogsteen hydrogen bonding. Because of hydrophobicity, guanine tetrads in water stack on top of each other to form helicoidal nanowires (the G-quadruplex). More recently, lipophilic guanilic derivatives (lipoGs), characterized by different substituents on the sugar moiety or by the replacement of the sugar with less hydrophilic units, have been synthesized and it has been proved that they exhibit a rich supramolecular chemistry in organic solutions. The self-assembly of a lipophilic derivative of (5'S)-5',8-cyclo-2'-deoxyguanosine, a mutagenic and replication blocker product formed by a hydroxyl radical attack against DNA, has been investigated. This derivative forms, with high fidelity, a dodecameric complex composed of three stacked G-quartets in the presence of strontium picrate. Hence, the molecule retains the ability of pristine guanosine to form G-quartet structures. This is the first example of a fully-anti lipophilic G-quadruplex. In-solution Small Angle Neutron Scattering (SANS) experiments have been performed on the 1-SrP2 complex in chloroform. Experiments, performed as a function of temperature, clearly suggest that heating does not modify the structure of the scattering particles, although the reduction of the scattering intensity indicates that some disaggregation process should occur when the temperature is increased.

New Sorgentina Fusion Source (NSFS) Experimental Facility Supporting Materials Research

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Within the framework of research and development on fusion technology, a 14 MeV neutron source has long been considered as a key facility to perform irradiation tests supporting design and licensing of DEMO reactor. In this context, New Sorgentina Fusion Source (NSFS) project has been proposed taking advantage of well-established D-T generators technology, properly scaled in order to design a bright neutron source of some $10^{1}5$ n/sec. It is based on multiple 200 keV deuterium and tritium ion beams, produced and accelerated by means of ion generators and extraction grid proven technology currently utilized in neutral injectors at large experimental tokamaks. Beams deliver several Amperes towards a deuterium-tritium enriched layer on a rotating target where fusion reactions take place. Tests on materials damage upon neutron irradiation are intended to be performed with the actual 14 MeV neutron spectrum typical of fusion reactors. NSFS project is intended to be carried out within national as well as international collaborations in order to provide a fusion-related neutron source but also a multipurpose facility. In present contribution, the main facility characteristics are highlighted along with expected irradiation performances.

D16 DIFFRACTOMETER AT THE ILL

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D16 is one of ILL's 2-axis cold neutron diffractometer. In terms of Q-space and Q-resolution, and nicely fills the gap between the small angle instruments and classical diffractometers.

Because of its special characteristics, D16 remains unequalled for the study of a wide range of systems in biology, physics and material science.

Its specifications have been optimized for the study of structures with relatively large periodicities of about 5 nm. These include large unit-cell lamellar organizations such as membranes or clays, two-dimensional membrane and surface lattice structures, colloidal and liquid structures, magnetic systems with large fluctuations giving rise to satellite reflections very close to Bragg peaks or small-angle scattering.

The instrument geometry offers a variable vertical focussing which allow working in reflectivity or diffraction mode. The scattering geometry obtained with large, vertically oriented samples, profits the most from the large vertical cross section of the beam at the sample position. A high resolution SANS setup is used routinely in experiments requiring the 1% wavelength bandwidth and the high angular resolution of the instrument. In this presentation the new design, the major characteristics, performances and new directions of the instrument will be showed, as well as recent examples of research on D16.

CASE STUDY FOR A VIBRATIONAL SPECTROSCOPY INSTRUMENT AT THE EUROPEAN SPALLATION SOURCE

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Neutron vibrational spectroscopy is a well established experimental technique where elementary excitations, at relatively high frequency, are detected via inelastic neutron scattering. This technique attracts a high interest in a large fraction of the scientific community in the fields of chemistry, materials science, physics, and biology, since one of its main applications exploits the large incoherent scattering cross section of the proton, with respect to all the other elements, whose dynamics can be spectroscopically detected, even if dissolved in very low concentration in materials composed of much heavier atoms. We proposed a feasibility study for a Vibrational Spectroscopy Instrument (VSI) at the European Spallation Source ESS. The preliminary design calculations and the corresponding McStas simulation results for a possible ToF Inverted Geometry instrument are summarised.

THE CRG BRISP AT ILL

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The neutron Time-of-Flight BRIllouin SPectrometer BRISP for inelastic neutron scattering at small angles was developed and constructed at ILL's High Flux Reactor in the framework of an Italian-German Collaborating Reserach Group. BRISP aims at investigating a host of open scientific problems in the low-momentum region with relatively high incoming neutron energies. With this dedicated instrument, the high-frequency dynamics of atomic nuclei and electron spins is studied in rather different materials. In the first years of experimental activity BRISP has shown its capability in approaching and providing data in a variety of disordered and magnetic systems. Originally planned for the investigation of these kind of systems, BRISP has immediately found a natural experimental extension to the study of those systems that have attracted in recent years a growing interest in the scientific community e.g. confined liquids, glasses, and biological macromolecules. A presentation of the instrument will be provided together with the illustration of some recent highlights.

Partnership for Soft Condensed Matter

Y. Gerelli

Institut Laue - Langevin, Grenoble (F)

The Partnership for Soft Condensed Matter (PSCM) is a scientific and technical platform enabling ambitious large-scale Soft Matter research projects addressing challenges in nanomaterials, environmental and energy sciences, and biotechnology. The PSCM promotes the integrated exploitation of state-of-the-art neutron and synchrotron beamlines in combination with the most advanced laboratory techniques for the characterization of a wide spectrum of systems ranging from soft interfacial thin films to complex multi-component bulk fluids.

The PSCM offers on-site sample preparation and characterization facilities located in a new laboratory building that is physically connected to both ILL and ESRF experimental halls. The collaborative development of specialized sample environments and instruments enables cutting-edge experiments for the investigation of the structure and dynamics of bulk and interfacial soft matter systems, such as self-assembled nanomaterials and bio-inspired hierarchical structures.

In the poster the possible activities, the user support programs and example of research carried out in the new PSCM laboratories will be explained.

LET COLD NEUTRON MULTI-DISK CHOPPER SPECTROMETER AT ISIS

T. Guidi

ISIS Facility, Rutherford Appleton Laboratory, Chilton Didcot, Oxfordshire, OX11 0QX, UK

LET is a cold neutron multi-chopper spectrometer for the study of dynamics in condensed matter. It resides within the new second target station at the ISIS facility. It has been optimized to take advantage of the high fluxes of cold neutrons this target station was designed for. Features include a wide dynamic range with large neutron fluxes over incident energies from $0.5 - 30$ meV and excellent energy resolutions of up to 8 μeV are possible. The detector array at completion will consist of a massive π steradians of position sensitive 4 m long ^{3}He tubes. The instrument was also designed to take extreme sample environment, with the 9 T wide opening magnet and dilution fridge being the most popular ones. To make use of the long 100 ms time frame LET runs in multi repetition rate mode with typically around 5 incident energies per frame covering the full dynamic range.

The ISIS pulsed neutron source

T. Guidi

ISIS Facility, Rutherford Appleton Laboratory, Chilton Didcot, Oxfordshire, OX11 0QX, UK

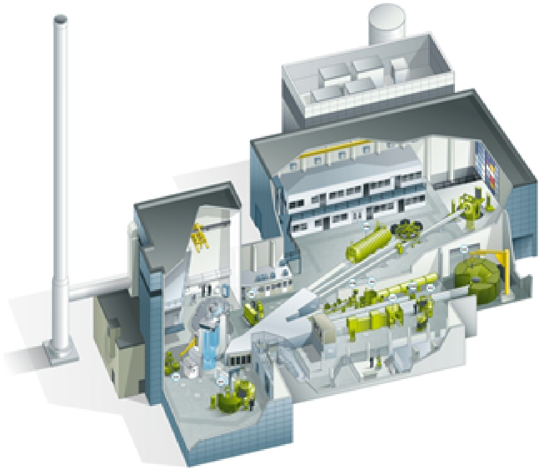
ISIS is a world-leading centre for research in the physical and life sciences at the Rutherford Appleton Laboratory near Oxford in the United Kingdom. Our suite of neutron and muon instruments give unique insights into the properties of materials at the scale of atoms. ISIS supports a national and international community of more than 3000 scientists. Research areas range from clean energy and the environment, pharmaceuticals and health care, through to nanotechnology and materials engineering, catalysis and polymers, and on to fundamental studies of materials.

BER II Neutron Facility at HZB

T. Gutberlet

Helmholtz Zentrum Berlin GmbH

The Helmholtz-Zentrum Berlin für Materialien und Energie HZB operates two large scale research facilities: the upgraded medium flux research reactor BER II on Lise-Meitner-Campus in Berlin-Wannsee and the third generation synchrotron source BESSY II on Wilhelm-Conrad-Röntgen-Campus in Berlin-Adlershof. In addition, it is home to a number of state-of-the-art on-site laboratories and user facilities. All these research facilities are designed to serve researchers from universities, foreign research institutions and industry. The BER II neutron facility offers a complete set of continuously renewed instruments for neutron scattering and imaging with thermal as well as cold neutrons. Unique research opportunities are provided due to a continuously expanded world-leading sample environment for complex neutron experiments under extreme conditions, e.g. at highest magnetic fields and lowest temperatures. Both thermal and cold neutrons are available. At current beamtime at 14 instruments is offered, including world class single crystal and powder diffractometers, two small angle neutron scattering instruments, two tomography and radiography stations, two reflectometers, the cold three axis spectrometers FLEXX and the extreme environment diffractometer EXED. On-site laboratories are available for sample preparation and supporting measurements. Beam time is offered by open proposal calls two times per year. Access to BER II is supported for European user by the NMI3-II access program. Further information is available at our webpages `www.helmholtz-berlin.de/user/index_en.html`



The thermal backscattering spectrometer CRG-IN13 at ILL

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The thermal backscattering spectrometer IN13 at the Institut Laue Langevin, is operated by a French-Italian Collaborative Research Group (CRG). It works with thermal neutrons with wavelength 2.23 Å. The energy resolution, almost Q-independent, is of the order of 8 eV and the instrument fills the energy gap between IN10 or IN16 (1 eV) and IN5 at the ILL or MIBEMOL at the LLB (15 eV). In addition, the relatively high energy of the incident neutrons ($\sim$ 16 meV) facilitates spanning of a wide range of momentum transfer Q (≥ 4.9 Å^{-1}). IN13 is mostly devoted to the study of the dynamical features of macromolecular systems in the eV energy region. Even though, scientific applications of IN13 can be found in areas of material science, solid-state physics, geophysics and chemistry, IN13 is mainly devoted to life sciences.

So far, the domain of biological fields studied with neutrons on IN13 spans from the single amino acid (the smaller component of the protein primary sequence) to in vivo cells and recently even to cerebral tissue. Examples are here reported.

FUNCTIONALIZED ZnO NANOPARTICLES: A SUITABLE TOOL FOR INNOVATION IN OPTOELECTRONICS AND BIOSENSING

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Zinc oxide nanoparticles (ZnO NPs) present very attractive optical and electronic properties, which make them an interesting component in the development of novel materials for application as optoelectronic devices and sensors. Indeed ZnO is a semiconductor and ZnO NPs are characterized by an intense fluorescence in the visible region. Furthermore, ZnO NPs can be easily obtained through a wet chemical-method, they are considered green, since their low environmental impact, and certainly it is possible to develop a simple recycle protocol, which is fundamental for industrial application. Here we present the preparation and a structural characterization of two ZnO NPs based systems for application in optoelectronic and biosensing field.

Due to its direct wide band gap and its large exciton binding energy, zinc oxide is commonly employed in optoelectronics. However, ZnO shows poor absorption in the visible region, so that its potential application needs a combination with a suitable photosensitive molecule. In order to enhance the efficiency in Dye Sensitized Solar Cells (DSSCs) melanins biopolymers such polydopamine, in combination with metal oxide nanoparticles, have been recently proposed. In particular, we present a new functionalization procedure of ZnO NPs with polydopamine (ZnO NPs-PDA) pointing to obtain a 2D and potential 3D array, with the aim to design a novel material with improved optical and electrical properties for application as nanodiodes or potential active layer in a new generation of eco-friendly solar cells.

With the purpose to exploit further the unique properties of ZnO, we also synthesized a hybrid system composed by ZnO NPs and single walled carbon nanotubes (SWNTs), as a suitable biosensors and potential nanocarriers for drug delivery. Indeed, SWNTs, which consist of a single tube of graphene, are of special interest for their bright emission in the near and mid-infrared region, where the tissues are transparent. In order to improve the intensity of SWNTs fluorescence signal, we developed a synthesis protocol for coating SWNTs with ZnO NPs (SWNTs-ZnO NPs) and a subsequent functionalization procedure to stabilize the hybrid system in aqueous suspension.

The presented ZnO NPs based systems have been previously characterized combining different techniques. In particular, diffraction and scattering techniques, such as Small Angle Neutron Scattering and Small Angle X-ray Scattering, have been used to define the structure of the prepared samples. On the other hand, spectroscopic measurements have also been fundamental to characterize the optical and electronic properties of both ZnO NPs-PDA and SWNTs-ZnO NPs.

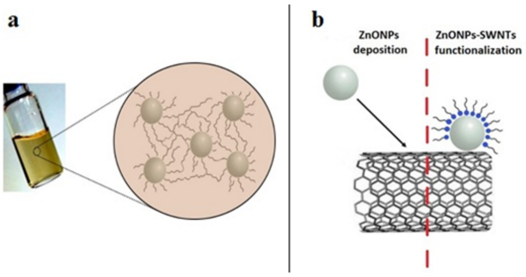

Figura 3: Schematic representation of ZnO NPs functionalized with polydopamine (panel a) and of functionalized ZnO NPs-SWNTs (panel b).

THE FRASCATI NEUTRON GENERATOR

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The Frascati Neutron Generator (FNG) is neutron source designed and realized at the Neutron Generator Laboratory of the ENEA Frascati Research Centre. The laboratory operates in the research and development framework of EFDA program for Magnetic Confinement Controlled Thermonuclear Fusion.

FNG produces almost monochromatic neutron with 2.5 MeV and 14 MeV energies exploiting fusion reactions using accelerated deuterons (up to 300 keV energy) impinging onto deuterium or tritium containing solid targets, respectively.

Intense yields can be achieved as high as 10^9 n/s for 2.5 MeV and $10^{1}1$ n/s for the 14 MeV. These yields, that can be tuned by modifying the deuteron current, allow different kind of irradiations to be performed:

- Cross sections measurements and neutron transport database validation through Benchmark and Mock-up irradiations for fusion neutronics study.
- Neutron induced materials activation.
- Calibration and characterization of fast neutron detectors.
- Single Event Effects in electronics.
- Neutron irradiation of biological samples.

Together with the neutron source the laboratory is equipped with calibrated High-Purity Germanium detectors (40% and 60% relative efficiencies) and a $\beta - \gamma$ coincidence detector.

An upgrade is foreseen to setup a thermal neutron irradiation station characterized by a high homogeneity over a surface of 50×50 cm^2 and an optimized Cd ratio to provide almost Maxwellian neutron spectrum. This facility, where both thermal neutrons and fast neutron can be available, will be exploited, for neutron detector characterization for different applications like He-replacement activity, homeland security, characterization of neutron instrumentation and components.

In this talk the main characteristics of FNG will be outlined, the research activity presented and future perspectives for the neutron users and developers community discussed.

^{3}HE-FREE TRIPLE GEM THERMAL NEUTRON DETECTOR

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A novel type of thermal neutron detector based on the gas electron multiplier (GEM) technology is presented in the framework of the research and development activity on the ^{3}He replacement for neutron detection. The device relies on a series of boron-coated alumina sheets placed perpendicularly to the incident neutron beam direction. A first prototype of the device mounting only four sheets was developed at INFN-Frascati and tested at the TRIGA reactor (ENEA-Casaccia) to assess its performances in terms of efficiency and dynamic range, being also corroborated by Monte Carlo simulations.

A new prototype version was tested on beam at the High Flux Isotope Reactor at the Oak Ridge National Laboratory (US) to assess its performance in terms of beam position resolution, efficiency and signal-to-background (S/B) ratio as compared to a 10 bar ^{3}He tube for sub-thermal neutrons. The obtained results, that are going to be presented in this contribution, demonstrate the effectiveness of the proposed detector configuration to achieve a good spatial resolution and, in the perspective, a higher thermal neutron efficiency, comparable to ^{3}He tubes typically used for diagnostic in nuclear reactors. Furthermore, the main issues to be addressed to reach the goal, mostly related to boron coating procedures and characterization, will be also pointed out.

IN8: THE HIGH FLUX THERMAL TRIPLE AXIS INSTRUMENT AT ILL

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IN8 is a high-flux thermal neutron three-axis spectrometer designed for inelastic measurements on single crystals over a wide range of energy and momentum transfer. IN8 is optimised for inelastic measurements with an energy transfer in the range of a few meV to about one hundred meV and, thanks to its 10^8 $\mathrm{n \cdot s^{-1} \cdot cm^{-2}}$ at the sample, it is used to investigate samples of small volume and weak inelastic response. In particular it has been widely employed to study weak magnetic excitations in superconductors and exotic magnetic materials, lattice vibrations in materials for energy applications and excitations in liquids.

The instrument works with the classical single detector setup, but it can also hosts the Flatcone multi-analyser detector system.

The incident wavelength selection is obtained through a double focusing monochromator, which has three faces equipped with PG002, Cu200 and bent perfect Si111 crystals, respectively. For special high-resolution experiments using a flat monochromator, Soller collimators are available.

The monochromator take-off angle varies in the range $10\,\mathrm{deg} < 2\theta_M < 90\,\mathrm{deg}$. The scattering angle at the sample position is in the range $0\,\mathrm{deg} < 2\theta_s < 120\,\mathrm{deg}$ independent of the monochromator take-off angle.

For the TAS configuration, PG002, Si111 and Cu111 analysers are used with a single type detector.

The instrument allows using a wide range of sample environment equipment such as high field magnets up to 10 T. For low scattering angle experiments the sample to analyzer distance can be increased to host a vacuum box to reduce air scattering.

X-RAY CRYSTALLOGRAPHY GIVES YOU THE FRAMES TO BUILD A BEAUTIFUL MOVIE

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X-ray crystallography is probably the most powerful tool to obtain a high-resolution picture of biomacromolecules and their complexes. It is also able to furnish indirect indications of global or local flexibility of these molecules. However, it often needs to be used in combination with different techniques, in particular with those that work on samples in solution and not at crystal state.

We extensively used X-ray crystallography to unveil the structural details of the recognition process between a biomedical relevant protein, human thrombin, and several oligonucleotidic aptamers[1-4]. Structural characterization by X-ray diffraction, together with a spectroscopic analysis, allowed us to define the effect that different ions have on the structure and flexibility of the aptamers, and in turn on their thrombin affinity and inhibition properties.

Recently, through a very detailed high-resolution structure of an all modified locked-nucleic-acid G-quadruplex, we derived interesting indications on the effect of modified nucleotides in quadruplex structure and stability and also obtained some cues to the possibility of designing LNA-based building blocks for nanotechnology[5].

Another fascinating topic is that of the ribonucleases (RNases) that present different properties depending on their structural features. On one hand, a long structural study, performed through a combination of crystallographic and docking analyses, allowed us to identify the structural determinants of antitumor activity in the dimeric BS-RNase, and to convert successfully the monomeric non-cytotoxic and non-immunogenic RNase A in a dimeric highly cytotoxic mutant[6]. On the other hand, starting from the crystal structure, we recently suggested that a different RNase mutant is able to form fibrils in solution, retaining its original fold and confirmed the formation of fibrils by atomic force microscopy [7].

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INES, THE ITALIAN NEUTRON EXPERIMENTAL STATION @ ISIS

A Scherillo

ISIS facility, STFC, UK & IPCF-CNR, Messina, Italy

INES is a neutron scattering instrument, built and managed by the Italian National Research Council (CNR) within the cooperation agreement with STFC, operational at the ISIS pulsed neutron source, UK.INES was built in 2005 and its user program run since 2006/2007.INES is a general purpose powder diffractometer and is mainly devoted to material characterisation (structure refinement and phase analysis), cultural heritage studies and equipment tests. Beamtime is available to users of any nationality. An overview of the instrument is presented, with some examples to better describe the research performed by the INES user community.

SOLVENT EXTRACTION: LIQUID-LIQUID INTERFACES BY X-RAY AND NEUTRON REFLECTIVITY

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Liquid-Liquid (LL) or solvent extraction is a separation process [1] which is based on the transfer of a solute from a solution 1 towards an immiscible phase 2, the contact with which can be enhanced by emulsification. In other terms, it is a partitioning method used to separate compounds based on their relative solubility in two different immiscible liquids, usually water and an organic solvent. The solubility is enhanced via the use of complexing molecules (an extractant) either hydrophilic or lipophilic, that are slightly amphiphilic [2,3]. The ultimate aim for application is to develop a selective transfer more cheaply and more quickly, although a trade-off always exists between selectivity and kinetics. The extraction mechanisms as well as their kinetics at molecular scale across the interface are still poorly understood even if attempts have been made [4][5]. In any case, the hydrated or solvated species (as a function of the transfer direction) have to explore various crossing configurations - very often different from those existing in bulk - associated to energy barriers that determine a part of the kinetics. Several unknown variables are left to quantify the energy barrier of the ion sorption and desorption at the active interface and in a complex association with the extractant molecules [6]. In other words, the interfacial concentration and distribution (of ions and extractants) at equilibrium but also out of equilibrium have to be determined during the ion transfer process. Since the extraction process depends both on the extractant concentration in oil and ions in water, our purpose is to measure interfacial structure changings, trying to be sensitive both at ions (Neodymium and Lithium Nitrate) and extractanct (DMDBTDMA or Diamide).For that purpose we designed a new cell both for x-Ray and Neutron reflectivity tested for experiments at ESRF (Grenoble) and J-PARC (Japan). On one side, with x-Ray, the low contrast between diamide and oil gives us access to informations about the ions-diamide interaction at interface. On the contrary, with neutron reflectivity, we can work with isotopic substitution, obtaining more informations about extractant distribution in bulk and at interface.

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