

SOCIETÀ ITALIANA DI SPETTROSCOPIA NEUTRONICA



XXVII CONGRESSO ANNUALE SISN
ITALIAN NEUTRON SCATTERING CONFERENCE 2016

Ancona & Senigallia
29 Giugno-1 Luglio 2016

BOOK OF ABSTRACTS

In memoria di Elisa Barzagli

Indice

Programma	8
Neutroni per la Scienza	18
Abstract dei talk	25
Abstract dei poster	40
Un ricordo di Elisa Barzagli	52
Indice degli autori	54

Programma

Mercoledì 29 Giugno

Università Politecnica delle Marche, Ancona
Dipartimento di Scienze della Vita e dell'Ambiente
Aula Azzurra

Neutroni per la Scienza Sessione speciale del XXVI Congresso SISN

14.30

REGISTRAZIONE

15.15

BENVENUTO

Perché i neutroni?

Una panoramica di applicazioni dei neutroni per la ricerca

Chairman: Debora Berti

15.10

Materials Science with Neutrons: a Toolkit

Giovanni Bruno

15.30

Non-destructive quantitative determination of the manufacturing methods of ancient Indian swords through neutron diffraction and neutron tomography

Francesco Grazzi

15.50

Addressing tumor cells with temperature tunable nanogel surfaces: when SANS helps in understanding the mechanism

Gaio Paradossi

16.10

From the dynamics of biological macromolecules to the structure of the ribosomal machinery: the contribution of Neutrons to Biology

Maria Grazia Ortore

16.30 – 17.00

COFFEE BREAK

Keynote lecture

Chairman: Alessio De Francesco

17.00

Presentazione della Società Italiana di Spettroscopia Neutronica

Paolo Mariani

17.15

Understanding Water with Neutron Scattering

José Teixeira

Neutroni per la Scienza è una sessione speciale del XXVII Congresso Annuale SISN – INSC2016, proposta per promuovere l'uso e le potenzialità delle tecniche di scattering neutronico in diversi ambiti di ricerca. La partecipazione a questa sessione è libera.

Giovedì 30 Giugno

Biblioteca Civica, Senigallia
Sala Congressi

8.30

REGISTRAZIONE

8.50

APERTURA DEL XXVII CONGRESSO ANNUALE SISN & ITALIAN NEUTRON SCATTERING
CONFERENCE

Chairman: Francesco Spinozzi

9.00

Understanding the nanoparticle-protein complexes and their biological effects using neutrons

Francesca Baldelli Bombelli

9.20

Integrated Motions of Molecular Machines and Motors: Supramolecular Complexes and Networks Structures as seen by SANS

Giacomo Mariani

9.40

SANS study of alkylglycoside surfactants with oligomeric head-group: understanding of self-aggregation, and its implications for future applications

Federica Sebastiani

10.00

Diffusion of the Protein Bovine Serum Albumin in the Presence of the Trivalent Salt YCl_3 Studied by Neutron Backscattering

Marco Grimaldo

Sorgenti Future I

Chairman: Paolo Mariani

10.30

Sorgentina: un progetto per una sorgente nazionale neutroni

Sandro Pace

10.50

Discussione

11.00 – 11.30

COFFEE BREAK

Chairman: Marco Maccarini

11.30

Development of in-situ neutron cells to investigate fundamental structural mechanisms involved in Li-ion (Na-ion) batteries

Tatiana Renzi

11.45

Thermodynamics of protein-nanoparticle interactions: a SANS study

Paolo Moretti

12.00

Neutron Study of Magnetic and Electric Ordering in the Metal-Organic Framework $[\text{NH}_4][\text{Mn}(\text{HCOO})_3]$

Lidia Mazzuca

12.15

An insight on the manifold dynamics found in liquid methanol

Stefano Bellissima

12.30

PRANZO & POSTER SESSION

Al Vecchio Mercato del pesce, Senigallia

Sorgenti Future II

Chairman: Paolo Mariani

14.30

Overview dei progetti Italiani per la neutron science a ESS

Cirino Vasi (TbC)

14.45

T-REX: A Time-of-flight Reciprocal space Explorer for the future European Spallation Source

Andrea Orecchini

15.00

The VESPA spectrometer at ESS

Giuseppe Gorini

15.15

SANS Detectors

Giuseppe Gorini

15.30

Efficient Shielding for the European Spallation Source: Borated concrete and ceramic B4C tiles

Francesco Grazi

15.45

USANS for SANS instruments: the project OPUS for Loki@ESS

Claudia Mondelli

16.00

Discussione

16.15 - 16.45

COFFEE BREAK

16.45 - 19.00

ASSEMBLEA DEI SOCI SISN

*L'Assemblea inizierà con un ricordo di Elisa Barzagli,
giovane ricercatrice e socia SISN recentemente scomparsa.*

20.30

CENA SOCIALE

**Ristorante Pagaia
Molo di Levante, Senigallia**

Venerdì 1 Luglio

Biblioteca Civica, Senigallia
Sala Congressi

Chairman: Gino Paduano

9.00

Direct observation of finite size effects in chains of antiferromagnetically coupled spins

Tatiana Guidi

9.20

Portraying entanglement between molecular qubits with four-dimensional inelastic neutron scattering

Elena Garlatti

9.40

Crystal dynamics of neptunium dioxide

Luigi Paolasini

10.00

The Multi-Blade ^{10}B -based neutron detector for high intensity neutron reflectometry at ESS

Francesco Piscitelli

10.20

Developing thermal neutron facilities with uniform, extended irradiation area

Antonino Pietropaolo

10.40 - 11.10

COFFEE BREAK

11.15 - 12.30

VERSO IL 2020: IL FUTURO DELLA NEUTRONICA ITALIANA VERSO ESS

Tavola rotonda moderata da Paolo Mariani.

12.30

CONCLUSIONI E SALUTI

Posters

Development of in-situ neutron cells to investigate fundamental structural mechanisms involved in Li-ion (Na-ion) batteries

Tatiana Renzi

Neutron diffraction measurement of thermal residual stresses in sintered metal-ceramic composites

Fabrizio Fiori

Development of a pulse-shape analysis method for neutron solid-state detectors

Giacomo Mauri

Investigation on suitability of consolidant and protective products on Sicilian calcarenites using Small Angle Neutron Scattering

Simona Raneri

Search for the elusive magnetic state of hexagonal iron. Antiferromagnetic $\text{Fe}_{71}\text{Ru}_{29}$ alloy

Francesco Sacchetti

Measurement of correlation functions of free neutrons. Characterization of the experimental set-up.

Pietro Tozzi

An insight on the manifold dynamics found in liquid methanol

Stefano Bellissima

Neutron Study of Magnetic and Electric Ordering in the Metal-Organic Framework $[\text{NH}_4][\text{Mn}(\text{HCOO})_3]$

Lidia Mazzuca

Thermodynamics of protein-nanoparticle interactions: a SANS study

Paolo Moretti

Neutroni per la Scienza

MATERIALS SCIENCE WITH NEUTRONS: A TOOLKIT

G. Bruno

University of Potsdam, Institute of Physics and Astronomy, and BAM, Bundesanstalt für Materialforschung und -prüfung, Berlin Germany.

"Neutrons are a powerful tool" say the neutron scientists. However the use of neutrons remains sometimes disconnected from the practical problems of Materials Science, and facilities themselves are seen as ivory towers.

In this presentation, I will give an overview of the modalities of access to Large Scale facilities, and show a couple of examples on how neutron scattering data on engineering materials can be used as a tool to understand, and even tailor, materials performance.

In order for this to happen, it is clear that neutron data need to be

1. Acquired under the most relevant condition possible
2. Coupled to other experimental techniques
3. Capitalized by means of proper simulations and data analysis

Point 1- calls for an intense use and the development of top-notch of in-situ techniques; Point 2- means that the sole use of neutron data will not lead to any solution of a global problem; All points above hint to the fact that access to neutron sources is not routine, and therefore it is imperative to search ways to make neutron data rentable for the material science and industrial research community.

NON DESTRUCTIVE QUANTITATIVE DETERMINATION OF THE MANUFACTURING METHODS OF ANCIENT INDIAN SWORDS THROUGH NEUTRON DIFFRACTION AND NEUTRON TOMOGRAPHY

F. Grazzi¹, A. De Francesco², E. Barzagli¹, F. Salvemini³, A. Scherillo⁴, B. Schillinger⁵, A. Williams⁶, D. Edge⁶

¹Consiglio Nazionale delle Ricerche, Istituto dei Sistemi Complessi, Sesto Fiorentino (FI), Italy.

²Consiglio Nazionale delle Ricerche, Istituto Officina dei Materiali c/o OGC, Grenoble, France.

³Bragg Institute, Australian Nuclear Science and Technology Organisation (ANSTO), Lucas Heights NSW, Australia.

⁴Science and Technology Facility Council, ISIS Neutron Source, Didcot, UK.

⁵Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universitaet Muenchen, Garching, Germany.

⁶The Wallace Collection, London, UK

Indian blades were famed in literary and history accounts since Greek and Roman time for their attractive combinations of ductility and high impact hardness, together with a stunning superficial pattern. Over time the Indian arms technology passed to the Persians and from them to Arabs who spread it through the Middle East and lately Europe. Unfortunately, the ancient manufacturing technique is a lost art and the date of the last blades produced with the highest-quality feature is uncertain, but is probably around the 18th century. The analysis of the micro-structural features of ancient Indian swords has been carried out by neutron diffraction and neutron tomography. The results provide a clear identification of the different types of steel used to produce such weapons. Among them, only a small proportion of the large number of swords produced in India were made of the hypereutectoid textured steel, namely *wootz*, also known as "Damascus steel". The others present characteristics very similar to those of European swords produced in the same period, including composites of low and high carbon steels assembled together and in the application of thermal treatments.

Neutron diffraction analysis was applied to a group of eight swords and their micro-structural and compositional characteristics were all identified non-destructively, revealing the use of strongly differentiated construction materials in producing the swords, from low carbon steel for the cheapest weapons to the highly refined and peculiar micro-structural features of at least one kind of *wootz* steel. Four of these swords were analyzed using neutron tomography in both white beam and in energy selective configurations permitting the determination of the spatial distribution of the iron and steel components within the swords and the size and orientation of the ferrite and cementite grains in the *wootz*.

These results are an important starting point in leading to comprehension of the metal selection and the forging procedures used to produce swords made of *wootz*. This is a further proof of the validity of the use of neutron techniques for the non-destructive yet quantitative characterization of ancient metal artifacts.

ADDRESSING TUMOR CELLS WITH TEMPERATURE TUNABLE NANOGEL SURFACES: WHEN SANS HELPS IN UNDERSTANDING THE MECHANISM

G. Paradossi¹, F. Domenici¹, B. Cerroni¹, L. Oddo¹, M. Telling², S. Rogers²

¹Dipartimento di Scienze e Tecnologie Chimiche, Università di Roma Tor Vergata, Rome, Italy.

²ISIS Facility, STFC, Rutherford Appleton Laboratory, Chilton, Didcot, UK.

In the design of a polymer hydrogel, poly(*N*-isopropylacrylamide), (p(NiPAAm)), moiety is often included as thermoresponsive component. Its lower critical solubility temperature (LCST) displayed in water is close to the physiological temperature and is used to obtain a "smart" structural responsivity, consisting in the hydrogel shrinking [1]. However, in a hybrid network, the presence of other components is equally important in determining the overall hydrogel behaviour. In this respect, hyaluronic acid (HA) has recently gained considerable attention as co-participant with p(NiPAAm), to assemble a novel type of hybrid nanogels showing intriguing thermoresponsive features. HA is known to be stable, biodegradable, and able to interact preferentially with tumour cells overexpressing integrins, thus adding a huge therapeutic value to the construct. In this framework, we recently realized nanosized, chemically cross-linked, HA-p(NiPAAm) hydrogel particles, in which HA is derivatized with azide-bearing side chains and "clicked" with a telechelic p(NiPAAm) bearing terminal alkyne groups synthesized by reversible addition-fragmentation chain transfer, RAFT [2]. Photon correlation and z-potential spectroscopies show the nanogel particles have a size of ~ 150 nm at 25 °C. Moreover, below the LCST the particles' surface is biphasic. However, around 31°C, rather than shrinking, the surface properties of the HA-pNiPAAm particles change. A dramatic shift in the zeta-potential of the particles is observed, suggesting a prevalence of HA at the surface and a transfer of p(NiPAAm) to the core of the material. This process has been followed by combining small angle neutron scattering (SANS) and atomic force microscopy (AFM). SANS scattering law at high *q*'s and a power spectral density study of AFM images allows to follow the reshaping of the surface of the nanogel particles. Such a reorganizational process of the nanogel surface has remarkable potential in terms of selective delivery of anticancer drugs in tumour cells. In particular, the delivery of doxorubicin drug via the HA/p(NiPAAm) nanogel particles reduced by 50% the viability of HT 29 tumour cells with respect to healthy fibroblasts NIH3T3.

[1] K.L. Hamner, C.M. Alexander, K. Coopersmith, D. Reishofer, C. Provenza, M.M. Maye, *ACS Nano* **7**, 7011 (2013).

[2] B. Cerroni, S.K. Pasale, A. Mateescu, F. Domenici, L. Oddo, F. Bordi, G. Paradossi, *Biomacromolecules* **16**, 1753 (2015).

FROM THE DYNAMICS OF BIOLOGICAL MACROMOLECULES TO THE STRUCTURE OF THE RIBOSOMAL MACHINERY: THE CONTRIBUTION OF NEUTRONS TO BIOLOGY

M.G. Orto

Dipartimento di Scienze della Vita e dell'Ambiente, Università Politecnica delle Marche, Ancona, Italy.

The use of neutrons to investigate biological molecules arises from their properties: they are uncharged particles able to interact directly with nuclei, they can be penetrative and non-destructive, and they especially present the ability to detect hydrogen and differentiate it from its stable isotope deuterium. The last property is enhanced by the fact that biology is rich in water and hydrogen, and this allows to exploit the differential sensitivity of neutrons to this element and its major isotope. Small Angle Neutron Scattering about 40 years ago let to determine the location of RNA inside ribosomal subunits and opened a window onto promising opportunities to deeply investigate biological structures, even in combination with other experimental techniques involving X-rays.

Neutrons are also unique tools to investigate dynamical behavior of proteins, DNA, lipids and their hydration shells because hydrogen has a very large incoherent scattering cross section, and so is the main origin of this type of scattering signal measured from biological samples. Several biological questions can be faced by using neutrons, because they can provide structural characterizations spanning from angstroms to microns and dynamic information from picoseconds to microseconds. This overview describes some successful applications of available techniques based on neutrons to biomolecular systems and would present possible outcomes for the next future.

UNDERSTANDING WATER WITH NEUTRON SCATTERING

J. Teixeira

Laboratoire Léon Brillouin (CEA/CNRS), CEA-Saclay, Gif-sur-Yvette, France.

Omnipresent and almost only liquid on the Earth surface, water has unique properties which are not yet fully understood. Among the many unusual thermodynamic properties, even the explanation of the density maximum at 277 K is a matter of debate. Because the anomalous behaviour is more pronounced at low temperature, many experiments were performed in the temperature region below the melting point, where the liquid state is metastable. However, nucleation of the solid phase prevents experiments below about 250 K, far above the glass transition temperature (135 K). Thus, a large domain of temperature of the order of 100 K remains totally unknown. As a consequence, many speculative models have been and are proposed, from the simple two-phase mixture originally proposed by Roentgen till some recent simulations based on effective potentials describing the hydrogen bond molecular interaction. Some of them generate unexpected singularities, for example, low temperature critical points.

Among several other scattering techniques, the contribution of neutron scattering is particularly important. QENS and SANS results will be presented within the context of the present debate about the postulated coexistence of two phases in liquid water. Arguments will be given in favour of a model of a homogeneous liquid with large density fluctuations. It will be shown that mixture models are incompatible with both thermodynamic data and the local structure of the liquid.

Instead, the anomalous temperature dependence of water properties can be explained by the strong temperature dependence of the number of intermolecular hydrogen bonds and of their characteristic lifetime, which can be evaluated by neutron scattering. A more detailed description of the complex mechanisms of hydrogen bond formation is the present more important open question to be solved in the long way of the knowledge of liquid water.

Abstract dei talk

UNDERSTANDING THE NANOPARTICLE-PROTEIN COMPLEXES AND THEIR BIOLOGICAL EFFECTS USING NEUTRONS

F. Baldelli Bombelli

Department of Chemistry, Material and Chemical Engineering G. Natta, Politecnico di Milano, Milano, Italy.

The fast development of nanotechnology and growing use of nanomaterials in different fields increased the chance to voluntary or accidental exposure of the human body to nanoparticles (NPs), which could in some cases lead to adverse effects for health. Thus, a clear understanding of the interaction of NPs with the biological matter is crucial and not only limited to nanomaterials specifically developed for biomedical applications. Most of the difficulties encountered by the nanoformulations to reach the clinics are not only due to issues related to the scaling-up of the production methodologies, but also to the complexity of the interaction between NPs and biological matter. The first contact between NPs and living organisms occurs in the biological fluid, where protein-NP complexes are immediately formed, then these protein corona (PC) NPs will first interact with the cell membrane. Thus, understanding PC NP-cell interactions is a critical step to design safer and more efficient NPs as well as to predict possible toxicity effects. In this work the use of neutrons to study the formation of PC NPs and their effect on lipid membranes will be shown: in particular how neutron-based techniques can represent optimal complementary methodologies to better understand the interaction of nanomaterials and biological matter.

AN INSIGHT ON THE MANIFOLD DYNAMICS FOUND IN LIQUID METHANOL

S. Bellissima¹, F. Formisano², S. De Panfilis³, E. Guarini¹, U. Bafle⁴, M. A. González⁵

¹Dipartimento di Fisica e Astronomia, Università di Firenze, Italy.

²CNR-IOM, Grenoble, France.

³Centre for Life Nano Science IIT, Roma, Italy.

⁴CNR-ISC, Sesto Fiorentino, Italy.

⁵Institut Laue Langevin, Grenoble, France.

Methanol is a hydrogen-bonded liquid of enormous importance in pure and applied physics and chemistry, and is the object of innumerable studies. Yet, the fundamental aspects of its molecular dynamics are still known only to a very poor extent. The study of the collective dynamics is hindered by the weakness of the acoustic excitations, which has led to the wrong conclusion that sound modes propagate only in a surprisingly narrow range of small wave vector values. Exploiting the combination of molecular dynamics simulations and neutron Brillouin scattering measurements, methanol is shown, for the first time, to feature the normal viscoelastic behavior typical of a large variety of liquids. Besides this, however, two more excitations are detected in the molecular centre-of-mass dynamics structure factor, at frequencies, respectively, one lower and one higher than the acoustic frequency. The rich dynamics revealed by this study classifies methanol as a fluid partly similar to the most important hydrogen-bonded liquid: the water.

PORTRAYING ENTANGLEMENT BETWEEN MOLECULAR QUBITS WITH FOUR-DIMENSIONAL INELASTIC NEUTRON SCATTERING

E. Garlatti¹, T. Guidi², S. Ansbro^{3,4}, P. Santini¹, G. Amoretti¹, J. Ollivier³, H. Mutka³, G. Timco⁴, I.J. Vitorica-Yrezabal⁴, G.F.S. Whitehead⁴, R.E.P. Winpenny⁴, S. Carretta¹

¹Dipartimento di Fisica e Scienze della Terra, Università di Parma, Italy.

²ISIS facility, Rutherford Appleton Laboratory, Didcot, United Kingdom.

³Institut Laue-Langevin, Grenoble, France.

⁴School of Chemistry and Photon Institute, The University of Manchester, Manchester, United Kingdom.

Entanglement is a crucial resource for quantum information processing and its detection and quantification are of paramount importance in many areas of current research. Weakly-coupled molecular nanomagnets (MNM)s provide an ideal test bed for investigating entanglement between complex spin systems and are currently attracting increasing attention for quantum information processing. However, entanglement in these systems has only been experimentally demonstrated rather indirectly by macroscopic techniques or by fitting trial model Hamiltonians to experimental data. Recently, we have shown that dynamical correlations between individual spins in MNMs can be directly determined in a model-free approach through the four-dimensional inelastic neutron scattering technique [1].

Here we show that this technique can be exploited to demonstrate and quantify inter-ring entanglement in the eigenstates of a $(\text{Cr}_7\text{Ni})_2$ supramolecular dimer. We have found clear and peculiar modulations of the neutron cross section as a function of the components of the wavevector \mathbf{Q} , which are directly connected with spin-spin correlations and represent a sort of "portray" of the entanglement in the eigenstates of the system. By exploiting $(\text{Cr}_7\text{Ni})_2$ as a benchmark, we show the potential of this approach, which allows us to extract the concurrence in eigenstates of this dimer without diagonalizing its full Hamiltonian

[1] M.L. Baker *et al.*, Nature Phys. **8**, 906 (2012).

DIFFUSION OF THE PROTEIN BOVINE SERUM ALBUMIN IN THE PRESENCE OF THE TRIVALENT SALT YCl_3 STUDIED BY NEUTRON BACKSCATTERING

M. Grimaldo^{1,2}, F. Roosen-Runge², M. Hennig^{1,2}, F. Zanini², F. Zhang², M. Zamponi^{3,4}, N. Jalarvo^{3,5}, F. Schreiber², T. Seydel¹

¹Institut Laue-Langevin (ILL), Grenoble, France.

²Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany.

³Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH, Jülich, Germany.

⁴JCNS Outstation at the MLZ, Garching, Germany.

⁵Chemical and Engineering Materials Division, Neutron Sciences Directorate, and JCNS Outstation at the Spallation Neutron Source (SNS), Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States.

Proteins are macromolecules involved in a great number of processes essential for life, occurring in living cells together with other macromolecules at large volume fractions (molecular crowding) and larger assembled structures, as well as with different kinds of sugars and ions. Similar conditions can significantly influence protein dynamics [1–3]. In the simple case of one single type of negatively charged protein in solution, the presence of multivalent cations results in a rich phase behavior, characterized, amongst others, by protein aggregation –often related to neurodegenerative diseases–, liquid-liquid phase separation, and crystallization.

In this talk, we will present the results of experiments carried out at the backscattering spectrometer BASIS at the ORNL on the dynamics of bovine serum albumin (BSA) in D_2O in the presence of the multivalent salt YCl_3 [3]. A slowing down of the apparent diffusion coefficient of BSA molecules as a function of the number of cations per protein c_s/c_p in solution is found remarkably universal in c_p . The result is interpreted in terms of the theory of colloidal suspensions of patchy particles as a result of the semi-quantitative binding of Y_3^+ ions to specific sites on the protein surface leading to the formation of protein clusters with a cluster size distribution easily tunable by c_s/c_p .

[1] M. Grimaldo *et al.* J. Phys. Chem. B **118**, 7203–7209 (2014).

[2] M. Grimaldo *et al.* Phys. Chem. Chem. Phys. **17**, 4645–4655 (2015).

[3] M. Grimaldo *et al.* J. Phys. Chem. Lett. **6**, 2577–2582 (2016).

DIRECT OBSERVATION OF FINITE SIZE EFFECTS IN CHAINS OF ANTIFERROMAGNETICALLY COUPLED SPINS.

T. Guidi

ISIS facility, Rutherford Appleton Laboratory, United Kingdom.

Finite spin chains made of a few magnetic ions are the ultimate-size structures that can be engineered to perform spin manipulations for quantum information devices. Their spin structure is expected to show finite size effects and its knowledge is of great importance both for fundamental physics and applications. The experimental realization of finite spin chains has traditionally involved a top-down approach where an ideal infinite chain is "cut" into segments by introducing diamagnetic impurities. This procedure leads to an ensemble of chains with different lengths, containing a number of atoms with varying parity. Therefore the study of their magnetic behaviour and the effect on their magnetic properties associated with the parity of the chain is averaged out in the experimental measurements. A more flexible and controlled bottom-up approach is offered by the chemistry of antiferromagnetic molecular rings.

We have investigated the spin dynamics and local moment distribution of two prototypical members of this family of molecules, the homonuclear Cr_8 "closed" ring and the heteronuclear Cr_8Cd "open" ring. Their quantum spin dynamics has been fully unravelled using four-dimensional INS measurements and their microscopic spin structure has been quantitatively determined using polarized neutron diffraction. The results reveal finite-size effects depending on the boundary condition and the parity of the chains.

INTEGRATED MOTIONS OF MOLECULAR MACHINES AND MOTORS: SUPRAMOLECULAR COMPLEXES AND NETWORKS STRUCTURES AS SEEN BY SANS

G. Mariani¹, A. Goujon², E. Moulin², N. Giuseppone², E. Buhler¹

¹Matière et Systèmes Complexes (MSC) Laboratory University of Paris Diderot-Paris VII, UMR 7057
Bâtiment Condorcet, Paris, France.

²SAMS research group, Institut Charles Sadron, CNRS University of Strasbourg, Strasbourg, France.

Switchable functional molecules producing mechanical work constitute an active focus in nanotechnologies as they can be used for molecular-based devices and materials. The dynamic nature of mechanically interlocked molecules allows their components to undergo relative internal movements. However, the coupling of these components to transfer controlled motions from the monomer to the macroscopic scale is a challenge. Using metallo-supramolecular polymerization process, we have realized supramolecular polymer chains that are sufficiently long so that micrometric changes can be measured upon synchronization of thousands of contractions and extensions. We have demonstrated the contraction/extension of a single-chain supramolecular polymer based on a pH-responsive molecular rotaxane showing the synchronization of thousands of molecular machines [1]. However, further hierarchical organization of these single-chain polymers into higher-scale structures is required, as myofibrils do when packed in bundles of muscular fibers.

In this contribution, we report on the structural characterization of two new contractile supramolecular polymers. Two different approaches have been followed to form network-like structures similar to the bundles of muscular fibers [2,3]. In the first one additional capable side chains have been added to the monomers resulting in an additional interaction. In the second one, light-driven rotary motors have been integrated as mechanically active reticulation units. The structural changes have been investigated using SANS and light scattering. In both the cases, the curves show evidence of the formation of bundles of polymer chains. In the latter case, the mesh size of the network is ranging from 3 to 4.5 nm upon contraction, whereas heterogeneity size decreases from 450 (extended state) to 260 nm (contracted state).

[1] G. Du, E. Moulin, N. Jouault, E. Buhler, N. Giuseppone, *Angew. Chem. Int. Ed.* **51**, 12504-12508 (2012).

[2] Q. Li, G. Fuks, E. Moulin, M. Maaloum, M. Rawiso, I. Kubic, J. T. Foy, N. Giuseppone, *Nature Nanotech.* **10**, 161-165 (2015).

[3] A. Goujon, G. Du, E. Moulin, G. Fuks, M. Maaloum, E. Buhler, N. Giuseppone, *Angew. Chem. Int. Ed.* **55**, 703-707 (2016).

NEUTRON STUDY OF MAGNETIC AND ELECTRIC ORDERING IN THE METAL-ORGANIC FRAMEWORK $[\text{NH}_4][\text{Mn}(\text{HCOO})_3]$

L. Mazzuca¹, L. Cañadillas-Delgado², O Fabelo¹, J.A. Rodríguez-Velamazán^{1,3}, J. Rodríguez-Carvajal¹, G. De Munno⁴

¹Institut Laue Langevin, Grenoble, France.

²Centro Universitario de la Defensa, Zaragoza, Spain.

³Instituto de Ciencia de Materiales, Aragón, Spain. CSIC-Universidad de Zaragoza, Spain.

⁴Dipartimento di Chimica, Università della Calabria, Arcavacata di Rende, Italy.

The development and the characterization of new materials are key challenges in chemistry and physics. In particular metal-organic frameworks (MOFs) with multiferroic properties are still rare and very interesting due to the wide variety of structural architectures that can be obtained. In this study we focused on the porous crystalline material with general formula $[\text{X}][\text{M}(\text{HCOO})_3]$ where X is an amine counter-ion and M is a divalent metal. The compound is typically synthesized by reacting an organic ligand with a metal salt under solvo-thermal conditions or by slow evaporation or diffusion techniques. The chemical nature of the ligand (HCOO^-) plays a crucial role, being the smallest and simplest carboxylate it mediates the magnetic exchange interaction between the metal centres. The latter may also be governed by a template molecule, e.g. protonated amines [1]. Such a molecule, influence the formation of the material with its size effect, charge balance and its hydrogens bonding interacting with the anionic framework. The ammonium cation (NH_4^+) employed and accommodated in the cavities of the framework, can introduce functionalities such as ferroelectricity in coexistence with magnetism [2]. The $[\text{NH}_4][\text{Mn}(\text{HCOO})_3]$ compound crystallize in the hexagonal space group $P6_322$ at room temperature and it shows at 254 K a paraelectric to ferroelectric phase transition associated to a nuclear phase transition from $P6_322$ to $P6_3$, generated by order-disorder state of NH_4^+ cation [3]. In order to better understand the trigonal disorder of the cation, the high sensitivity of neutron diffraction has been significant for obtaining the refinement at the low temperature nuclear structure, and also to acquire an accurate model including the hydrogen atoms positions. Regarding the magnetic properties, the experimental data indeed evidenced an antiferromagnetic ordering at 8 K [3]. The goal of this work has been to explore the structural and magnetic phase transitions and to perform the nuclear and magnetic structure determination below T_N using single crystal neutron diffraction technique.

[1] J.M. M. Lawler, P. Manuel, A. L. Thompson and P. J. Saines, Dalton Trans. **44**, 11613 (2015).

[2] G.-C. Xu, W. Zhang, X.-M. Ma, Y.-H. Chen, L. Zhang, H.-L. Cai, Z.-M. Wang, R.-G. Xiong, S. Gao, J.Am. Chem. Soc. **133**, 14948-14951 (2011).

[3] Z. Wang, B. Zhang, M. Kurmoo, K. Inoue, H. Fujiwara, T. Otsuka, H. Kobayashi and M. Kurmoo, Inorg. Chem. **46**, 437-445 (2007).

THERMODYNAMICS OF PROTEIN–NANOPARTICLE INTERACTIONS: A SANS STUDY

P. Moretti¹, G. Ceccone², P. Ghigna³, C. Ferrero⁴, G. Campanella⁵, F. Spinozzi¹

¹DiSVA Department, Università Politecnica delle Marche.

²European Commission DG JRC –IHCP Unit Nanobiosciences Ispra.

³Department of Chemistry, University of Pavia, Pavia, Italy.

⁴European Synchrotron Radiation Facility, Grenoble, France. ⁵Weill Cornell Medical College, New York, NY, USA.

Although it is generally accepted that nanoparticles (NP) in contact with a biological medium are covered with a layer of proteins, there are still several open questions concerning the interaction mechanisms between NP and protein [1]. To address this issue, we report on a SANS experiment performed at LLB (PACE instrument) on gold nanoparticles (NPs) synthesized with sodium citrate and dissolved in D₂O in the presence of human serum albumin (HSA). The NPs diameter was 30 nm and the gold concentration was 4 mM. Several samples were investigated at HSA concentrations up to 0.018 mM.

SANS curves were analyzed with the GENFIT software [2] by modeling the NPs as polydispersed three-density levels spheres with an average radius of 15 nm coated, a first layer of citrate and a second layer composed by water and HSA. The form factor of unbound HSA proteins was calculated on the basis of available protein database files.

The composition of the second layer is ruled out by a thermodynamic equilibrium that describes the binding between a HSA molecule (P) and an association site (S) in the first citrate layer, according to the relation $P+S\rightarrow PS$. A thermodynamic model has been developed and integrated into the software, which allows determining the fraction of sites occupied by the protein as a function of the protein concentration. Hence, a simultaneous analysis of all SANS curves has been carried out by fitting each curve as a linear combination of the form factor of NPs and that of HSA with the relative populations calculated on the basis of the thermodynamic model.

The most important result of this study is the determination of the free energy of the association of a protein molecule to a site on the NP.

[1] I. Lynch, A. Salvati and K. A. Dawson, *Nature Nanotechnology* **4**, 546, (2009).

[2] F. Spinozzi, C. Ferrero, M.G. Ortore, A. De Maria Antolinos and P. Mariani, *J. Appl. Cryst.* **47**, 1132–1139 (2014).

CRYSTAL DYNAMICS OF NEPTUNIUM DIOXIDE

L. Paolasini¹, P. Maldonado², P. M. Oppeneer², T.R. Forrest¹, A. Prodi³, N. Magnani⁴, A. Bosak¹, G.H. Lander⁴, R. Caciuffo⁴

¹European Synchrotron Radiation Facility (ESRF), Grenoble, France.

²Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden.

³CNR-ISM, Montelibretti, Italy.

⁴European Commission, JRC-ITU, Karlsruhe, Germany.

The dispersion relation for normal modes of vibration propagating along high-symmetry lines in NpO_2 at room temperature has been determined measuring the coherent one-phonon scattering of X-rays from a ~ 1.2 mg single-crystal specimen. The results are compared against ab initio phonon dispersion simulations computed within the first-principles density functional theory in the generalized gradient approximation plus Hubbard U correlation (GGA+U) approach, taking into account third-order anharmonicity effects in the quasi-harmonic approximation. Good agreement with the experiment is obtained for calculations with an on-site Coulomb parameter $U = 4$ eV and Hund's exchange $J = 0.6$ eV. Thermal expansion, heat capacity, thermal conductivity, phonon linewidth, and thermal phonon softening are calculated and compared with available experiments. Data collected at 10 K suggest the occurrence of anomalies associated with vibrational and dispersive magnetic multipole excitations.

DEVELOPING THERMAL NEUTRON FACILITIES WITH UNIFORM, EXTENDED IRRADIATION AREA

R. Bedogni¹, J.M. Gómez-Ros^{1,3}, M.V. Intriaini², M. Lorenzoli², A. Pietropaolo⁴, M. Pillon⁴,
A. Pola², D. Sacco^{1,5}, A. Sperduti^{4,1}

¹INFN-LNF Laboratori Nazionali di Frascati, Frascati, Italy.

²Politecnico di Milano, Dipartimento di Energia, Milano, Italy.

³CIEMAT, Madrid, Spain.

⁴ENEA, Dip. Fusione e Tecnologie per la Sicurezza Nucleare, Frascati, Italy. ⁵INAIL-DPIA, Monteporzio Catone, Italy.

In the framework of the NEURAPID collaboration (INFN CSN5, 2014–2016), a new type of radionuclide source-based thermal neutron irradiation facility for was conceived.

The design includes of a large irradiation cavity (in the order of 30–40 cm in diameter and 50 cm in height in height), which is separated from the source by means of a polyethylene shadowing object. Taking advantage of multiple scattering of neutrons with the walls of this cavity, the moderation process is especially effective and allows obtaining useful thermal fluence rates in the order of $1.4 \times 10^{-4} \text{ cm}^{-2} \text{ s}^{-1}$ per unit emission rate. This is higher than in traditional designs, where the useful thermal neutron beam is the leakage field from a large moderating block embedding one or more sources. Irradiation planes parallel to the cavity bottom can be identified. After a brief general discussion of three practical facilities operating at INFN-LNF Frascati (ETHERNES), ENEA Frascati (HOTNES) and Politecnico di Milano (ESTHER), a detailed presentation of the preliminary results obtained on the HOTNES facility will be presented.

THE MULTI-BLADE ^{10}B -BASED NEUTRON DETECTOR FOR HIGH INTENSITY NEUTRON REFLECTOMETRY AT ESS

F. Piscitelli¹, R. Hall-Wilton²

¹European Spallation Source ERIC, Lund, Sweden.

²Mid-Sweden University, Sundsvall, Sweden.

The Multi-Blade is a Boron-10-based detector conceived to face the challenge of the counting rate capability arising from the neutron reflectometry at the European Spallation Source (ESS). The current detector technology is reaching fundamental limits in counting rate capability and position resolution.

The problem with count rates is a general one, and the ESS solution could potentially be applied to existing instruments at other neutron sources.

The work on the Multi-Blade began in 2011 at the Institut Laue-Langevin (ILL) where two technology prototypes were built and tested showing promising results. The European Union is now sponsoring the Multi-Blade detector through the BrightnESS project that aims to realise detectors optimized for these high rates.

The Multi-Blade design has been improved and a new demonstrator has been built and tested within the collaboration of ESS, Lund University and the Hungary's WIGNER research center for physics.

It has been shown that aside from the improvement in counting rate capability, the Multi-Blade design also decreases the spatial resolution by about a factor three over state-of-the-art helium-3-based reflectometer detectors.

These and other results including the path ahead for this project will be presented.

The Multi-Blade design is one of the favored as a development path to be pursued for reflectometry at ESS.

DEVELOPMENT OF IN-SITU NEUTRON CELLS TO INVESTIGATE FUNDAMENTAL STRUCTURAL MECHANISMS INVOLVED IN LI-ION (NA-ION) BATTERIES

M. Bianchini^{1,2,3,4}, T. Renzi^{1,2,3,4}, C. Masqueliera^{1,4}, L. Croguennec^{3,4}, E. Suard¹

¹Institut Laue-Langevin ILL, Grenoble, France.

²Laboratoire de Réactivité et Chimie des Solides, CNRS-UMR 7314, Université de Picardie Jules Verne, Amiens, France.

³CNRS, Univ. Bordeaux, ICMCB, UPR 9048, Pessac, France. ⁴RS2E, Réseau Français sur le Stockage Electrochimique de l'Energie, FR CNRS 3459, Amiens, France.

In the last decade the quest to improve Li-ion batteries followed a great number of different paths: not only new materials were looked for and designed, but also analysis techniques were developed and improved considerably to allow scientists to unravel the electrochemical cycling mechanisms. In-situ techniques recently proved to be remarkably useful tools to understand the behavior of Li-ion batteries [1] and custom made electrochemical cells for in-situ studies of Li-ion batteries were developed [2,3]. For instance, a (Ti,Zr)-based electrochemical cell [4] was recently designed at ILL, that allowed to follow in-situ and operando the structural modifications (new metastable phase formations, solid solutions, changes in crystallinity, etc.) associated with the reversible insertion/extraction of alkali cations from the positive and/or negative electrodes of Li-ion (Na-ion) batteries. This cell was specifically designed to provide, using liquid deuterated electrolyte, reliable electrochemical data and neutron powder diffraction data of sufficient quality to succeed in performing reliable Rietveld structural refinements [4,5].

A promising alternative to flammable organic electrolyte-based batteries is all-solid state batteries, which are gaining a lot of interest as they have less safety issues. We are thus now developing a new cell to be used for dry ceramic all-solid state batteries operating between 300 K and 600 K, which will inaugurate a new axis of research in our laboratories.

[1] M. Morcrette, Y. Chabre, G. Amatucci, J. B. Leriche, C. Masquelier, J. M. Tarascon, *Electrochim. Acta* **47**, 3137 (2002).

[2] F. Rosciano, M. Holzapel, W. Scheifele, P. Novak, *J. Applied Crystallography* **41**, 690 (2008).

[3] M. Roberts, J. J. Biendicho, S. Hull, P. Beran, T. Gustafsson, G. Svensson, K. Edstrom, *J. Power Sources* **226**, 249 (2013).

[4] M. Bianchini, J. B. Leriche, J. L. Laborier, L. Gendrin, E. Suard, L. Croguennec, C. Masquelier, *J. Electrochem. Soc.* **160**, A2176 (2013).

[5] M. Bianchini, L. Croguennec, E. Suard, C. Masquelier, *J. Phys. Chem. C* **118**, 25947 (2014).

SANS STUDY OF ALKYLGLYCOSIDE SURFACTANTS WITH OLIGOMERIC HEAD-GROUP: UNDERSTANDING OF SELF-AGGREGATION, AND ITS IMPLICATIONS FOR FUTURE APPLICATIONS

F. Sebastiani^{1,2}, S. Ulvenlund¹

¹CR Competence AB, Chemical Centre, Lund, Sweden.

²Physical Chemistry Department, Chemical Centre, Lund, Sweden.

The increased effort to preserve the environment has driven extensive research toward the identification of surfactants that are nontoxic, biodegradable, and synthesized from sustainable resources. Alkylglycosides with oligomeric head-groups promise to meet these demands. This novel class of surfactants have been specifically designed to ensure biocompatibility and controlled biodegradability, and hence lend themselves to applications within the area of in vivo controlled release.

Our study focused on a surfactant with C₁₆ alkyl chain, and 8 glucose units in the head-group (C₁₆G₈). Since the functionalities and possible applications of C₁₆G₈ can compete with the widely used Polysorbate 80, we investigated thoroughly the self-aggregation mechanism. We characterised the system with several techniques, such as light scattering, both static (SLS) and dynamic (DLS), NMR, SAXS and SANS. The complementary use of neutrons and x-rays was crucial to determine the structure of the aggregates, since the contrast between the glucose chain and the alkyl chain differs when probed with x-rays and neutrons.

We will discuss the effect of temperature and concentration on the size and shape of the aggregates and, furthermore, the effect of different anomeric configurations. The combination of these techniques allowed us to reveal the features of this novel sugar surfactant and build a fundamental knowledge related to its potential for application.

Abstract dei poster

AN INSIGHT ON THE MANIFOLD DYNAMICS FOUND IN LIQUID METHANOL

S. Bellissima¹, F. Formisano², S. De Panfilis³, E. Guarini¹, U. Bafle⁴, M. A. González⁵

¹Dipartimento di Fisica e Astronomia, Università di Firenze, Italy.

²CNR-IOM, Grenoble, France.

³Centre for Life Nano Science IIT, Roma, Italy.

⁴CNR-ISC, Sesto Fiorentino, Italy.

⁵Institut Laue Langevin, Grenoble, France.

Methanol is a hydrogen-bonded liquid of enormous importance in pure and applied physics and chemistry, and is the object of innumerable studies. Yet, the fundamental aspects of its molecular dynamics are still known only to a very poor extent. The study of the collective dynamics is hindered by the weakness of the acoustic excitations, which has led to the wrong conclusion that sound modes propagate only in a surprisingly narrow range of small wave vector values. Exploiting the combination of molecular dynamics simulations and neutron Brillouin scattering measurements, methanol is shown, for the first time, to feature the normal viscoelastic behavior typical of a large variety of liquids. Besides this, however, two more excitations are detected in the molecular centre-of-mass dynamics structure factor, at frequencies, respectively, one lower and one higher than the acoustic frequency. The rich dynamics revealed by this study classifies methanol as a fluid partly similar to the most important hydrogen-bonded liquid: the water.

NEUTRON DIFFRACTION MEASUREMENT OF THERMAL RESIDUAL STRESSES IN SINTERED METAL–CERAMIC COMPOSITES

F. Fiori¹, M. Basista², S. Nosewicz², J. Rojek², W. Weglewski²

¹Università Politecnica delle Marche, Di.S.C.O., Ancona (Italy).

²IPPT, Polish Academy of Sciences, Warsaw (Poland).

In manufacturing of metal–ceramic composites by hot pressing of powders, local thermal residual stresses (TRS) are typically generated in the matrix and in the reinforcement during cooling from a high sintering temperature to room temperature, mainly due to different coefficients of thermal expansion of the matrix and the dispersed reinforcement. TRS, especially if tensile, may cause microcracking inside the matrix, on ceramic–metal interfaces and inside reinforcement grains affecting the mechanical properties of the composite such as elastic constants and tensile strength. Furthermore, TRS play an essential role on crack propagation as they can change the local state of stress at the interface and, thus, contribute positively or negatively to the bridging stresses in the metal ligament.

In the framework of a research aiming to an experimental–numerical investigation of the effect of TRS on the fracture behavior of metal–ceramic bulk composites, neutron diffraction measurements were carried out at the E3 diffractometer of the Helmholtz–Zentrum für Materialien und Energie, Berlin (HZB). The measured TRS will be used as input data for the numerical models of the TRS effect on the macroscopic fracture toughness. In particular, in this work the results on sintered NiAl/Al₂O₃ specimens are presented, with different reinforcement contents and with different sintering parameters (pressure and sintering time).

DEVELOPMENT OF A PULSE-SHAPE ANALYSIS METHOD FOR NEUTRON SOLID-STATE DETECTORS

G. Mauri¹, F. Sacchetti^{1,2}, C. Petrillo^{1,2}, F. Casinini²

¹Dipartimento di Fisica e Geologia, Università di Perugia, Perugia, Italia.

²CNR-IOM c/o Dipartimento di Fisica e Geologia, Perugia, Italia.

Current gas detectors used to reveal thermal and cold neutron have a high efficiency but are limited both in spatial and time resolution. To overcome this point, one possible solution is represented by solid-state detectors that have been developed since few years.

A typical device is made-up of a neutron converter coupled to a sensor and can achieve good time and space resolution still maintaining a high efficiency. A prototype based on a Gadolinium foil converter and a silicon micro-strip sensor was tested at the Institut Laue Langevin (ILL, Grenoble, France). The main feature of absorption process of neutrons in Gd is the production of conversion electrons with a probability of about 80%. Furthermore this process does not produce heavy ions that can damage the silicon sensor, but the conversion mechanism causes a x-ray emission resulting in a strong background component. To solve this issue a pulse-shape analysis of the recorded signal is required.

The analysis algorithm fits data points with a shape function, representing the theoretical signal originated by the neutron conversion mechanism. A first implementation of such a method leads to an efficiency of about 30%. This value can be improved by refining the code used for analysis. To this aim, we have implemented a simulation system that reproduces real data to test the analysis code, reaching a performance of almost 100%. The final goal is to build a compact programmable detector with an on board real-time analysis.

NEUTRON STUDY OF MAGNETIC AND ELECTRIC ORDERING IN THE METAL-ORGANIC FRAMEWORK $[\text{NH}_4][\text{Mn}(\text{HCOO})_3]$

L. Mazzuca¹, L. Cañadillas-Delgado², O Fabelo¹, J.A. Rodríguez-Velamazán^{1,3}, J. Rodríguez-Carvajal¹, G. De Munno⁴

¹Institut Laue Langevin, Grenoble, France.

²Centro Universitario de la Defensa, Zaragoza, Spain.

³Instituto de Ciencia de Materiales, Aragón, Spain. CSIC-Universidad de Zaragoza, Spain.

⁴Dipartimento di Chimica, Università della Calabria, Arcavacata di Rende, Italy.

The development and the characterization of new materials are key challenges in chemistry and physics. In particular metal-organic frameworks (MOFs) with multiferroic properties are still rare and very interesting due to the wide variety of structural architectures that can be obtained. In this study we focused on the porous crystalline material with general formula $[\text{X}][\text{M}(\text{HCOO})_3]$ where X is an amine counter-ion and M is a divalent metal. The compound is typically synthesized by reacting an organic ligand with a metal salt under solvo-thermal conditions or by slow evaporation or diffusion techniques. The chemical nature of the ligand (HCOO^-) plays a crucial role, being the smallest and simplest carboxylate it mediates the magnetic exchange interaction between the metal centres. The latter may also be governed by a template molecule, e.g. protonated amines [1]. Such a molecule, influence the formation of the material with its size effect, charge balance and its hydrogens bonding interacting with the anionic framework. The ammonium cation (NH_4^+) employed and accommodated in the cavities of the framework, can introduce functionalities such as ferroelectricity in coexistence with magnetism [2]. The $[\text{NH}_4][\text{Mn}(\text{HCOO})_3]$ compound crystallize in the hexagonal space group $P6_322$ at room temperature and it shows at 254 K a paraelectric to ferroelectric phase transition associated to a nuclear phase transition from $P6_322$ to $P6_3$, generated by order-disorder state of NH_4^+ cation [3]. In order to better understand the trigonal disorder of the cation, the high sensitivity of neutron diffraction has been significant for obtaining the refinement at the low temperature nuclear structure, and also to acquire an accurate model including the hydrogen atoms positions. Regarding the magnetic properties, the experimental data indeed evidenced an antiferromagnetic ordering at 8 K [3]. The goal of this work has been to explore the structural and magnetic phase transitions and to perform the nuclear and magnetic structure determination below T_N using single crystal neutron diffraction technique.

[1] J.M. M. Lawler, P. Manuel, A. L. Thompson and P. J. Saines, Dalton Trans. **44**, 11613 (2015).

[2] G.-C. Xu, W. Zhang, X.-M. Ma, Y.-H. Chen, L. Zhang, H.-L. Cai, Z.-M. Wang, R.-G. Xiong, S. Gao, J. Am. Chem. Soc. **133**, 14948-14951 (2011).

[3] Z. Wang, B. Zhang, M. Kurmoo, K. Inoue, H. Fujiwara, T. Otsuka, H. Kobayashi and M. Kurmoo, Inorg. Chem. **46**, 437-445 (2007).

THERMODYNAMICS OF PROTEIN–NANOPARTICLE INTERACTIONS: A SANS STUDY

P. Moretti¹, G. Ceccone², P. Ghigna³, C. Ferrero⁴, G. Campanella⁵, F. Spinozzi¹

¹DiSVA Department, Università Politecnica delle Marche.

²European Commission DG JRC –IHCP Unit Nanobiosciences Ispra.

³Department of Chemistry, University of Pavia, Pavia, Italy.

⁴European Synchrotron Radiation Facility, Grenoble, France. ⁵Weill Cornell Medical College, New York, NY, USA.

Although it is generally accepted that nanoparticles (NP) in contact with a biological medium are covered with a layer of proteins, there are still several open questions concerning the interaction mechanisms between NP and protein [1]. To address this issue, we report on a SANS experiment performed at LLB (PACE instrument) on gold nanoparticles (NPs) synthesized with sodium citrate and dissolved in D₂O in the presence of human serum albumin (HSA). The NPs diameter was 30 nm and the gold concentration was 4 mM. Several samples were investigated at HSA concentrations up to 0.018 mM.

SANS curves were analyzed with the GENFIT software [2] by modeling the NPs as polydispersed three-density levels spheres with an average radius of 15 nm coated, a first layer of citrate and a second layer composed by water and HSA. The form factor of unbound HSA proteins was calculated on the basis of available protein database files.

The composition of the second layer is ruled out by a thermodynamic equilibrium that describes the binding between a HSA molecule (P) and an association site (S) in the first citrate layer, according to the relation $P+S \rightarrow PS$. A thermodynamic model has been developed and integrated into the software, which allows determining the fraction of sites occupied by the protein as a function of the protein concentration. Hence, a simultaneous analysis of all SANS curves has been carried out by fitting each curve as a linear combination of the form factor of NPs and that of HSA with the relative populations calculated on the basis of the thermodynamic model.

The most important result of this study is the determination of the free energy of the association of a protein molecule to a site on the NP.

[1] I. Lynch, A. Salvati and K. A. Dawson, *Nature Nanotechnology* **4**, 546, (2009).

[2] F. Spinozzi, C. Ferrero, M.G. Ortore, A. De Maria Antolinos and P. Mariani, *J. Appl. Cryst.* **47**, 1132–1139 (2014).

NEUTRON DIFFRACTION MEASUREMENT OF THERMAL RESIDUAL STRESSES IN SINTERED METAL–CERAMIC COMPOSITES

F. Fiori¹, M. Basista², S. Nosewicz², J. Rojek², W. Weglewski²

¹Università Politecnica delle Marche, Di.S.C.O., Ancona (Italy).

²IPPT, Polish Academy of Sciences, Warsaw (Poland).

In manufacturing of metal–ceramic composites by hot pressing of powders, local thermal residual stresses (TRS) are typically generated in the matrix and in the reinforcement during cooling from a high sintering temperature to room temperature, mainly due to different coefficients of thermal expansion of the matrix and the dispersed reinforcement. TRS, especially if tensile, may cause microcracking inside the matrix, on ceramic–metal interfaces and inside reinforcement grains affecting the mechanical properties of the composite such as elastic constants and tensile strength. Furthermore, TRS play an essential role on crack propagation as they can change the local state of stress at the interface and, thus, contribute positively or negatively to the bridging stresses in the metal ligament.

In the framework of a research aiming to an experimental–numerical investigation of the effect of TRS on the fracture behavior of metal–ceramic bulk composites, neutron diffraction measurements were carried out at the E3 diffractometer of the Helmholtz–Zentrum für Materialien und Energie, Berlin (HZB). The measured TRS will be used as input data for the numerical models of the TRS effect on the macroscopic fracture toughness. In particular, in this work the results on sintered NiAl/Al₂O₃ specimens are presented, with different reinforcement contents and with different sintering parameters (pressure and sintering time).

INVESTIGATION ON SUITABILITY OF CONSOLIDANT AND PROTECTIVE PRODUCTS ON SICILIAN CALCARENITES USING SMALL ANGLE NEUTRON SCATTERING

G. Barone¹, P.P. Lottici², P. Mazzoleni¹, G. Predieri³, S. Raneri¹, J. Teixeira⁴

¹Department of Biological Geological and Environmental Sciences, University of Catania, Catania, Italy.

²Department of Physics and Earth Sciences University of Parma, Parma, Italy.

³Department of Chemistry, University of Parma, Parma, Italy.

⁴Laboratoire Léon Brillouin (CEA/CNRS), CEA/Saclay, Gif-sur-Yvette, France.

One of the main issues related to the conservation of building stones is the use of suitable consolidants and protective treatments. Crucial features in their efficiency evaluation are aspects such as penetration depth and distribution inside the stone pore network, often difficult to evaluate using standard test routine. As it is well known, neutrons are a useful probe to obtain structural information of materials. For example, by performing small angle scattering experiments, information about the size, the number density and the correlation between components of a sample can be obtained. Taking advantage from these aspects, in this study SANS has been used to investigate the spatial distribution of some nano-structured and hybrid consolidants and protective products applied on calcarenites quarried and used as building and replace stone in Sicily, named Assoro and Sabucina Stones (Central Sicily). Measurements have been carried out on PAXY instrument (LLB, France) on 1 mm thick treated stone slices, using contrast matching methods in order to eliminate the contribution of the stone matrix and better discriminate the added products. The results provided useful structural information on the employed products, demonstrating the existence of different arrangements inside the porous structure of the solid matrix. Such diverse structural features influence the capability of the products to properly preserve masonry, which is of great importance for applications in the field of Cultural Heritage conservation sciences.

DEVELOPMENT OF IN-SITU NEUTRON CELLS TO INVESTIGATE FUNDAMENTAL STRUCTURAL MECHANISMS INVOLVED IN LI-ION (NA-ION) BATTERIES

M. Bianchini^{1,2,3,4}, T. Renzi^{1,2,3,4}, C. Masqueliera^{1,4}, L. Croguennec^{3,4}, E. Suard¹

¹Institut Laue-Langevin ILL, Grenoble, France.

²Laboratoire de Réactivité et Chimie des Solides, CNRS-UMR 7314, Université de Picardie Jules Verne, Amiens, France.

³CNRS, Univ. Bordeaux, ICMCB, UPR 9048, Pessac, France. ⁴RS2E, Réseau Français sur le Stockage Electrochimique de l'Energie, FR CNRS 3459, Amiens, France.

In the last decade the quest to improve Li-ion batteries followed a great number of different paths: not only new materials were looked for and designed, but also analysis techniques were developed and improved considerably to allow scientists to unravel the electrochemical cycling mechanisms. In-situ techniques recently proved to be remarkably useful tools to understand the behavior of Li-ion batteries [1] and custom made electrochemical cells for in-situ studies of Li-ion batteries were developed [2,3]. For instance, a (Ti,Zr)-based electrochemical cell [4] was recently designed at ILL, that allowed to follow in-situ and operando the structural modifications (new metastable phase formations, solid solutions, changes in crystallinity, etc.) associated with the reversible insertion/extraction of alkali cations from the positive and/or negative electrodes of Li-ion (Na-ion) batteries. This cell was specifically designed to provide, using liquid deuterated electrolyte, reliable electrochemical data and neutron powder diffraction data of sufficient quality to succeed in performing reliable Rietveld structural refinements [4,5].

A promising alternative to flammable organic electrolyte-based batteries is all-solid state batteries, which are gaining a lot of interest as they have less safety issues. We are thus now developing a new cell to be used for dry ceramic all-solid state batteries operating between 300 K and 600 K, which will inaugurate a new axis of research in our laboratories.

[1] M. Morcrette, Y. Chabre, G. Amatucci, J. B. Leriche, C. Masquelier, J. M. Tarascon, *Electrochim. Acta* **47**, 3137 (2002).

[2] F. Rosciano, M. Holzapel, W. Scheifele, P. Novak, *J. Applied Crystallography* **41**, 690 (2008).

[3] M. Roberts, J. J. Biendicho, S. Hull, P. Beran, T. Gustafsson, G. Svensson, K. Edstrom, *J. Power Sources* **226**, 249 (2013).

[4] M. Bianchini, J. B. Leriche, J. L. Laborier, L. Gendrin, E. Suard, L. Croguennec, C. Masquelier, *J. Electrochem. Soc.* **160**, A2176 (2013).

[5] M. Bianchini, L. Croguennec, E. Suard, C. Masquelier, *J. Phys. Chem. C* **118**, 25947 (2014).

SEARCH FOR THE ELUSIVE MAGNETIC STATE OF HEXAGONAL IRON. ANTIFERROMAGNETIC $\text{Fe}_{71}\text{Ru}_{29}$ ALLOY

C. Petrillo^{1,2}, P. Postorino³, A. Orecchini^{1,2}, F. Sacchetti^{1,2}

¹Dipartimento di Fisica e Geologia, Università di Perugia, Perugia, Italia

²CNR-IOM Unità di Perugia c/o Dipartimento di Fisica e Geologia, Perugia, Italia

³Dipartimento di Fisica, Sapienza-Università di Roma, Roma, Italia

The magnetic states of iron represent an important test case for the physics of magnetism because of the role in basic and applied science. Indeed, the presence of different crystallographic structures and different magnetic configurations in a very small range of the ground state energy makes iron critical for the development of first principle calculations. On the other hand, the geophysical importance of high pressure and temperature states of iron implies the need for a deeper knowledge of the properties of this element, which is the most diffused heavy element in the universe.

The *hcp* iron is the most elusive one, because it exists only at high pressure, although it is expected to be stable up to very high temperature. To investigate the magnetic state of an hexagonal Fe lattice, we performed a neutron diffraction experiment as a function of temperature on the *hcp* $\text{Fe}_{71}\text{Ru}_{29}$ disordered alloy. The hexagonal Fe lattice in this specific condition results to be antiferromagnetically aligned with a rather complex structure and a low magnetic moment. The temperature dependence suggests a Néel temperature $T_N = 124 \pm 10$ K, a value compatible with the low magnetic moment of $1.04 \pm 0.10 \mu_B$ obtained from the diffraction data, showing also a non-commensurate magnetic structure with magnetic moments probably aligned along the *c* axis.

The results are discussed in the light of theoretical findings and compared with those obtained for the Fe lattice in other compact environments, such as the *fcc* alloys of Fe-Ni, where Fe is ferromagnetic with high magnetic moment, and of Fe-Mn, where Fe is antiferromagnetic with a low magnetic moment. It is also observed that the atomic volume of the present alloy extrapolated to *hcp* iron is 11.30 \AA^3 , very close to that extrapolated for *fcc* iron in Fe-Mn alloys (11.35 \AA^3), but it is smaller than both ferromagnetic *bcc* iron (11.71 \AA^3) and ferromagnetic *fcc* iron extrapolated from Fe-Ni alloys (12.07 \AA^3).

These results suggest that a complex antiferromagnetic state in pure *hcp* Fe is possible, considering its presence in the $\text{Fe}_{71}\text{Ru}_{29}$ alloy, where Ru atoms are expected to reduce the possibility of a magnetic alignment.

MEASUREMENT OF CORRELATION FUNCTIONS OF FREE NEUTRONS. CHARACTERIZATION OF THE EXPERIMENTAL SET-UP.

P. Tozzi¹ and F. Sacchetti^{1,2}

¹Dipartimento di Fisica e Geologia, Università di Perugia, Perugia (Italy)

²CNR-IOM UOS Perugia c/o Dipartimento di Fisica e Geologia, Università di Perugia, Perugia (Italy)

Bell's Theorem states that no local and deterministic physical theory with hidden variable can reproduce the predictions of quantum mechanics. The theorem is considered as an important contribution to quantum mechanics, in particular its counterintuitive nature in the rejection of local realism. Over the years, many experiments were performed whose purpose was to confirm the local or non-local nature of the real physical world. This poster show an introduction to Bell's inequality and some of its implications accompanied by an overview of experiments, all based on the measurement of correlated photons. In 2011 he was made an innovative experiment using pairs of entangled particles, neutrons in the singlet state; this experiment will be run again with some changes to the set-up used. The changes were made due to the results obtained with the exposed work, whose main purpose was to study some characteristics of the experiment set-up and thus allow further analysis of the data already collected. We wanted to observe the ability to polarize a neutron beam by the two filters used in the experiment it is exposed a description of scattering due to them. We will also discuss and descript the measurement of the polarization of the neutron beam and the mapping of the magnetic field in which the experimental set-up is immersed in.

Un ricordo di Elisa Barzagli

Vividi occhi e dolce sorriso... ecco la primissima immagine che di Te affiora. Limpido è il ricordo del nostro primo incontro, come terso era il mattino di gennaio del mio primo giorno al CNR. Non mi conoscevi ancora, eppure Tu eri lì a darmi il benvenuto con lo spirito di chi accoglie un'amica di lunga data. Il tuo calore, la tua freschezza, la tua spontaneità dissiparono in pochi istanti i timori e i dubbi di chi, come me, si affacciava al nuovo... e mi sentii come fossi a casa.

Così, è vivido il ricordo di quando mi raccontasti, mentre aspettavamo l'esito di un esame, del tuo nuovo progetto per la laurea specialistica. Il tuo contagioso interesse ha senza dubbio marcato un importante bivio della mia vita. E dopo pochi mesi, eccomi lì a lavorare al tuo fianco, travolta dal tuo tangibile entusiasmo.

Elisa, hai reso lieta la quotidianità di questi anni trascorsi insieme, prima che colleghe, amiche. Quanto abbiamo condiviso tra e oltre le mura di quell'ufficio: esperimenti, scuole SISN, panico da presentazione a congressi, pranzi e biscotti del babbo, isterismi da scrittura tesi, sorrisi, lacrime, confidenze in corridoio, passeggiate per il centro a Prato, lezioni di dizione sui reciproci dialetti, sguardi complici, timori, speranze, sogni della vita professionale e privata... Un intreccio ed equilibrio che ha reso lavorare insieme un piacevole gioco.

Stimata collega per acutezza, intelligenza e passione. Non sei mai stata parca di consigli e aiuto. E questo non solo in ambito lavorativo. Col tuo solito fare gentile, quasi in punta di piedi, sei entrata nelle nostre vite. Come dicevi, tu e la tua splendida famiglia ci avete adottate.

Poi, come non farsi travolgere dalla tua passione per il nuoto sincronizzato? Ogni volta ti si illuminavano gli occhi e all'improvviso ti ritrovavi non so come a parlare fitto fitto di costumi ed ascoltare musiche per i balletti delle tue allieve; è ancora una misteriosa magia come riuscissi a piroettare leggiadra in acqua, il tuo elemento.

Determinata, sicura, instancabile, grintosa, caparbia, travolgente Eli. L'incredibile forza e coraggio con cui hai affrontato la tua ultima sfida sono estati esempio per tutti. Ma lo sai icché? Piccola grande Guerriera, questo male ti avrà portata via, ma il tuo forte spirito e il tuo grande amore per la vita saranno sempre vivi. Già, possiamo versare lacrime perché te ne sei andata troppo presto, oppure sorridere ripensando a quanto abbiamo condiviso.

Cara Amica, la tua assenza, rende ora più difficile il viaggio. Solievo sol porta la consapevolezza di quanto fortunato sia stato l'aver camminato insieme e vedere quanto ci hai lasciato.

Sit tibi terra levis

Floriana e Anna

Index

Baldelli Bombelli, Francesca, 11, 26

Bellissima, Stefano, 12, 16, 27, 41

Bruno, Giovanni, 9, 19

Fiori, Fabrizio, 16, 42, 46

Garlatti, Elena, 15, 28

Gorini, Giuseppe, 13

Grazzi, Francesco, 9, 13, 20

Grimaldo, Marco, 11, 29

Guidi, Tatiana, 15, 30

Mariani, Giacomo, 11, 31

Mauri, Giacomo, 16, 43

Mazzuca, Lidia, 12, 16, 32, 44

Mondelli, Claudia, 13

Moretti, Paolo, 12, 16, 33, 45

Orecchini, Andrea, 13

Ortore, Maria Grazia, 9, 22

Pace, Sandro, 12

Paolasini, Luigi, 15, 34

Paradossi, Gaio, 9, 21

Pietropaolo, Antonino, 15, 35

Piscitelli, Francesco, 15, 36

Raneri, Simona, 16, 47

Renzi, Tatiana, 12, 16, 37, 48

Sacchetti, Francesco, 16, 49

Sebastiani, Federica, 11, 38

Teixeira, José, 10, 23

Tozzi, Pietro, 16, 50

Vasi, Cirino, 13

COMITATO SCIENTIFICO

Debora Berti, Flavio Carsughi, Alessio De Francesco,
Emiliano Fratini, Yuri Gerelli, Marco Maccarini, Paolo Mariani,
Gino Paduano, Alessandro Paciaroni, Francesco Spinozzi e
Marco Zanatta.



Con il patrocinio di:

Photos by: M. Cassani,
G. Mariani & C. Pierpaoli.



Dipartimento di
Scienze Fisiche e
Tecnologie della Materia



UNIVERSITÀ
POLITECNICA
DELLE MARCHE



Comune di Serravalle