Società Italiana di Spettroscopia Neutronica

XXIX Congresso Annuale SISN
Italian Neutron Scattering Conference INSC2018

4-6 Luglio 2018
Parma

Centro Congressi S. Elisabetta
Campus Universitario Area Scienze
Università degli studi di Parma

COMITATO ORGANIZZATORE

Stefano Carretta, Antonio Deriu, Maria Teresa di Bari, Luigi Paduano, Daniele Pontiroli e Marco Zanatta.

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Programma

Mercoledì 4 Luglio 2018
Università di Parma, Campus Universitario Area Scienze
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OLTRE 30 ANNI DI COLLABORAZIONE ITALIANA CON ISIS NEUTRON AND MUON SOURCE (UK)

14.00 Registrazione

14.15 Benvenuto e saluti
Fabio Bruni, Presidente SISN
Roberto Fornari, Pro Rettore con delega per la Ricerca - Università di Parma

14.30 **Keynote lecture**

ISIS: PAST, PRESENT AND FUTURE
Robert McGreevy, ISIS-STFC

15.15 Neutron diffraction for cultural heritage studies: the Italian Neutron Experimental Station INES@ISIS
Antonella Scherillo, ISIS-STFC

15.45 When symmetry and neutrons help understanding materials properties
Fabio Orlandi, ISIS-STFC

16.15 Giornate Didattiche, Summer and Advanced SISN Schools
Eleonora Guarini, Università di Firenze

16.30 Coffee Break & Poster Session

17.00 Fingerprints of Mn12, the forefather of molecular nanomagnets
Paolo Santini, Università di Parma

17.30 Neutron techniques and the study of arms and armour
Alan Williams, The Wallace Collection

17.50 Carbon nanostructures for energy-storage applications
Daniele Pontiroli, Università di Parma

18.20 The analysis of some Indo-Persian daggers from the Wallace Collection at the Italian Neutron Experimental Station, ISIS, Didcot, and their results.
David Edge, The Wallace Collection

18.40 Conclusioni

Gli interventi in questa sessione saranno in inglese. La partecipazione alla sessione è libera.

Giovedì 5 Luglio 2018
Università di Parma, Campus Universitario Area Scienze
Centro Congressi S. Elisabetta

8.30 Registrazione

I SESSIONE SCIENTIFICA

9.00 Evidence of a low temperature dynamical transition in concentrated microgels
Andrea Orecchini, Università di Perugia

9.30 Can multiple neutron scattering be computed without knowing the scattering law?
Ubaldo Bafile, IFAC-CNR

9.50 Ice XVII: structural and dynamical properties of the new form of porous ice
Leonardo Del Rosso, IFAC-CNR

10.10 Anisotropy of Co^{II} transferred to the Cr_7Co polymetallic cluster via strong exchange interactions
Elena Garlatti, ISIS-STFC

10.30 Magnetic Exchange and Crystal Field excitations of asymmetric Lanthanide dimers: An INS insight
Riaz Hussain, Università di Parma

10.45 The effects of manufacturing processes on historical ceramic morphology studied by Small Angle Neutron Scattering
Sandro Zorzi, Università Ca' Foscari Venezia

11.00 Coffee break

II SESSIONE SCIENTIFICA

11.30 Directional insertion of cone-shaped channel protein in model membranes by neutron reflectometry and electrophysiology
Laura Cantù, Università di Milano

12.00 Physico-chemical insights into Cardiolipin-containing Lipid Bilayers
Giuseppe Vitiello, Università di Napoli "Federico II"

12.20 Neutron reflectivity of layers formed by nanoparticle-surfactant complexes at the oil/water interface
Davide Orsi, Università di Parma

12.40 Short-time self-diffusion of immunoglobulin under different crowding conditions
Marco Grimaldo, Institut Laue-Langevin

12.55 Presentazione XP Power
Simone Torti, XP Power (Italy)

13.10 PRANZO & POSTER SESSION

III SESSIONE SCIENTIFICA

14:30 Neutron and synchrotron-based techniques for material science
Barbara Rossi, Elettra Sincrotrone Trieste

14.50 Modelling Option USANS upgrade: the project OPUS for LoKI@ESS and the upgrade of D11@ILL
Claudia Mondelli, CNR-IOM

15.10 Irradiation facilities for neutron detector testing and calibration
Roberto Bedogni, INFN-LNF

15.30 The VESPA project: Phase I completed
Stefano Bellissima, IFAC-CNR

15:50 **UPDATE SUI PROGETTI ITALIANI PER ESS**

16.30 Coffee break

17.00 **ASSEMBLEA DEI SOCI SISN**

20.30 **CENA SOCIALE**
Ristorante “Il Cortile”,
Borgo Paglia 3, Parma

Venerdì 6 Luglio 2018
Università di Parma, Campus Universitario Area Scienze
Centro Congressi S. Elisabetta

IV SESSIONE SCIENTIFICA

9:00 Hydrogen Bond Length as a Key to Understanding Sweetness
Maria Antonietta Ricci, Università di Roma Tre

9.20 Trehalose Protectant Activity for peptide hydration
Michael Di Gioacchino, Università di Roma Tre

9.35 Neutron scattering on gelatin: relevance for analog modelling
Silvia Brizzi, Università di Parma

9.50 Neutron scattering for sustainable energy materials: investigations of proton dynamics in acceptor-doped barium zirconates
Daria Noferini, JCNS @ Heinz Maier-Leibnitz Zentrum

10.10 Hydrogen dynamics in complex borohydrides
Luca Silvi, Helmholtz Zentrum Berlin

10.30 On the slowing down of 14 MeV fusion neutrons: a spectrometry benchmark and future perspectives
Antonino Pietropaolo, ENEA

10.45 BRISP_X: a project for the upgrade of the BRISP spectrometer at the ILL
Ferdinando Formisano, CNR-IOM

11.00 Coffee break

11.30 **GLI ACCORDI CON ILL E ISS: C'È UN FUTURO PER LA NEUTRONICA ITALIANA?**

Tavola Rotonda moderata da **Fabio Bruni**.

13.00 **CONCLUSIONI E SALUTI**

POSTERS

- Probing Structure and Mobility of Proteins in the Amorphous State at Low Hydration
  Ester Chiessi, Università di Roma Tor Vergata

- The analysis of some Indo-Persian daggers from the Wallace Collection at the Italian Neutron Experimental Station, ISIS, Didcot, and their results.
  David Edge, The Wallace Collection

- In-situ gas-sorption neutron studies at ISIS
  Mattia Gaboardi, Elettra Sincrotrone Trieste

- Unravelling the origin of high temperature magnetic bistability in dysprosocenium by inelastic neutron scattering
  Emilio Macaluso, Università di Parma

- Upgrades at the high-resolution backscattering spectrometer SPHERES
  Daria Noferini, JCNS @ Heinz Maier-Leibnitz Zentrum

- Investigation on suitability of consolidant and protective products on Sicilian calcarenites using Small Angle Neutron Scattering
  Luca Silvi, Helmholtz Zentrum Berlin

- Neutron techniques and the study of arms and armour
  Alan Williams, The Wallace Collection

Invited talks

Directional insertion of cone-shaped channel protein in model membranes by neutron reflectometry and electrophysiology

L. Cantù[1], V. Rondelli[1], E. Del Favero[1], P. Brocca[1], G. Thiel[2], A. Moroni[3]

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Insertion of a small potassium (K^+) channel protein (Kcv_{MA-1D} and Kcv_{NTS}) [1,2] in model membranes has been investigated by neutron reflectometry. The profitable small size of the investigated channel allows to perform measurements on macroscopic single supported bilayers of DPPC and DMPC. Reflectometry was also performed on bilayer of DPPC floating over a DSPC supported one, thus on a physically decoupled bilayer system, dynamically free. Fully deuterated lipids were used in order to highlight the contribution of the naturally hydrogenated protein to the reflected spectrum. In this perspective also substitution of the hydrogenated chaperon molecules with deuterated phospholipids, was performed. The insertion of the overall asymmetric, truncated cone-shaped channel tetramer into membranes, was studied by following the change in the contrast profile of the membranes after protein incubation in solution, representing the transverse structure of the bilayer. Results underscore an asymmetry of the contrast profile, demonstrating a favorable directional insertion.

Parallel electrophysiology experiments on the electrical activity of the channel reconstituted in planar lipid bilayers with the same composition also demonstrate a preferential orientation of the channel. We can speculate that when functional read-outs by electrophisiology are not possible, reflectometry can be a useful technique for assessing the transmembrane orientation. Moreover, matching the two techniques on reconstituted single membrane, highlights a route to structure-function connection on channel-protein biophysics. [3]

[1] S. Gazzarrini, M. Kang, A. Abenavoli, G. Romani, C. Olivari, D. Gaslini, G. Ferrara, J. L. van Etten, M. Kreim, S. M. Kast, G. Thiel, A. Moroni, *Biochemical Journal* 2009, **420**, 295.

[2] S. Tayefeh, T. Kloss, G. Thiel, B. Hertel, A. Moroni and S. Kast, *Biochemistry* 2007, **46**, 4826A.

[3] V.Rondelli, E.Del Favero, P.Brocca, G.Fragneto, M.Trapp, L.Mauri, M.G.Ciampa, G.Romani, C.J.Braun, L.Winterstein, I.Schroeder, G.Thiel, A. Moroni, L. Cantu', BBA - General Subjects 1862 (2018) 1742–1750.

[4] Work partially supported by grant n. 695078 - noMAGIC, H2020-ERC-2015

Evidence of a low temperature dynamical transition in concentrated microgels

Marco Zanatta[1], Letizia Tavagnacco[2], Elena Buratti[3], Monica Bertoldo[3], Francesca Natali[4], Ester Chiessi[5], Andrea Orecchini[6,7], Emanuela Zaccarelli[2]

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2. *CNR-ISC and Department of Physics, Sapienza University of Rome, Piazzale A. Moro 2, 00185, Rome, Italy.*
3. *CNR-IPCF Istituto per i Processi Chimico-Fisici, Sede Secondaria di Pisa, Consiglio Nazionale delle Ricerche, Area della Ricerca, via G. Moruzzi 1, 56124 Pisa, Italy.*
4. *CNR-IOM, Operative Group in Grenoble (OGG), c/o Institut Laue Langevin, 6 rue Jules Horowitz, BP 156, 38042 Grenoble cedex 9, France.*
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6. *Department of Physics and Geology, University of Perugia, Via A. Pascoli, 06123, Perugia, Italy.*
7. *CNR-IOM c/o Department of Physics and Geology, University of Perugia, Via A. Pascoli, 06123, Perugia, Italy.*

A low-temperature dynamical transition has been reported in several proteins. Here we provide the first observation of a “protein-like” dynamical transition in non-biological aqueous environments. To this aim we exploit the popular colloidal system of poly-N-isopropylacrylamide (PNIPAM) microgels, extending their investigation to unprecedentedly high concentrations. Thanks to the heterogeneous architecture of the microgels, water crystallization is avoided in concentrated samples, allowing us to monitor atomic dynamics at low temperatures. By elastic incoherent neutron scattering and molecular dynamics simulations we find that a dynamical transition occurs at a temperature T_d~250 K, independently from PNIPAM mass fraction. However, the transition is smeared out on approaching dry conditions. The quantitative agreement between experiments and simulations provides evidence that the transition occurs simultaneously for PNIPAM and water dynamics. The similarity of these results with hydrated protein powders suggests that the dynamical transition is a generic feature in complex macromolecular systems, independently from their biological function.

When symmetry and neutrons help understanding materials properties

Fabio Orlandi[1]

1. *ISIS Pulsed Neutron Facility, STFC, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11-0QX, United Kingdom*

Physical properties in crystalline solids are constrained and governed by the crystal symmetry. Indeed the influence of crystal symmetry is not only limited to the tensor properties through the Neumann's principle [1] and the Curie's law [2], but affect crystal excitations as well as the electronic band structures. It thus becomes clear that a precise and deep knowledge of the nuclear and magnetic symmetry is pivotal to understand, predict and engineer the material macroscopic properties. Neutron diffraction is the leading technique to study nuclear and magnetic structure of crystalline materials. In the talk, examples from different areas of physics, namley topological materials [3], multiferroics [4,5] and magnetocalorics [6], will be presented showing how the use of the WISH diffractometer at the ISIS facility, together with a detailed symmetry analysis helped understanding the materials peculiar physical properties.

[1] Neumann, F. (1885).
[2] Curie, P. J. Phys. **3**, 393–415 (1894).
[3] Schoop, L. M. *et al.* Sci. Adv. **4**, (2018).
[4] Li, M.-R. et al. Nat. Commun. **8**, 2037 (2017).
[5] Orlandi, F. *et al.* Inorg. Chem. **55**, 4381–4390 (2016).
[6] Orlandi, F. *et al.* in preparation (2018).

Carbon nanostructures for energy-storage applications

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and M. Riccò[1]

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2. *Elettra-Sincrotrone Trieste, Basovizza, Trieste, Italy*
3. *European Synchrotron Radiation Facility, Grenoble, France*
4. *Institut Laue Langevin, Grenoble, France*
5. *The Bragg Institute, Australian Nuclear Science and Technology Organisation, Kirrawee, NSW, Australia*

Nowadays, the urgency on the global scale to quickly switch to renewable sources strongly requires boosting the performances of the current energy-storage systems. Carbon-based materials appear rather promising for this purpose, thanks to their unique mechanical, electronic and structural properties and to their intrinsic environment-friendly character.

in the last years, the research at the Carbon Nanostructures Laboratory of the University of Parma has been mainly focused on the identification of new fullerene and graphene-based materials for energy-storage applications, either as solid-state hydrogen absorbers, or as components of novel lithium, sodium and magnesium ionic batteries, namely anodes and solid electrolytes, or again as electrodes in supercapacitors.

During this research, neutron scattering investigation revealed to be a valuable tool for a deeper understanding of the physics of these new systems. High resolution and high flux neutron powder diffraction, also coupled with synchrotron data, allowed to disentangle the complex crystalline structure of different alkali/alkali earth intercalated fullerides and to follow their phase evolution upon in-situ hydrogen absorption. On the other hand, quasielastic and inelastic neutron spectroscopy has been extensively employed to study the small alkali diffusion in the fullerene matrix, or the interaction of hydrogen with defects in differently functionalized graphene materials.

Fingerprints of Mn12, the forefather of molecular nanomagnets

A. Chiesa,[1, 2] T. Guidi,[3] S. Carretta,[1] S. Ansbro,[4] G. A. Timco,[4] I. Vitorica-Yrezabal,[4] E.Garlatti,[1] G. Amoretti,[1] R. E. P. Winpenny,[4] and P. Santini[1]

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3. *ISIS facility, Rutherford Appleton Laboratory, Didcot, UK*
4. *School of Chemistry, University of Manchester, UK*

The discovery of magnetic bistability in Mn12 more than 20 years ago marked the birth of molecular magnetism, an extremely fertile interdisciplinary field and a powerful route to create tailored magnetic nanostructures. However, the difficulty to determine interactions in complex polycentric molecules often prevents their understanding. Mn12 is an outstanding example of this difficulty: although it is the forefather and the most studied of all molecular nanomagnets, an unambiguous determination even of the leading magnetic exchange interactions was still lacking.

By using the LET spectrometer at ISIS, we managed to measure the inelastic cross-section for single crystals over large portions of the energy-wavevector space, thus obtaining a faithful portray of spin fluctuations on the space- and time-scales characterizing the internal dynamics of the magnetic core. This information allowed us to pinpoint the eigenstates of the spin Hamiltonian, and to univocally identify the values of exchange constants for the first time.

These results demonstrate the power of four-dimensional inelastic neutron scattering as an unrivalled tool to characterize magnetic clusters, and motivate the synthesis of new polycentric nanostructures, where the set of interactions is optimal for studying specific fundamental issues or for applications.

Highlight talks

The VESPA project: Phase I completed

Stefano Bellissima[1], Leonardo Del Rosso[1], Daniele Colognesi[1]
& the VESPA group

1. *Istituto di Fisica Applicata "Nello Carrara", Via Madonna del Piano 10, 50019 Sesto Fiorentino (FI).*

VESPA is one of the inelastic instruments of the ESS suite. In particular, it is the only spectrometer which is fully dedicated to Neutron Vibrational Spectroscopy (NVS) for chemical and material science applications. Thanks to the high resolution and flux in the energy range of interest, i.e. the so-called "fingerprint region", VESPA will produce world-leading science in NVS field.

The project has recently reached an important goal: the conclusion of Phase I, i.e. the Preliminary System Design phase, and is now preparing to start the next Phase.

Neutron diffraction measurements with a high-efficiency GEM side-on ^{10}B-based thermal neutron detector

Gerardo Claps [1], Antonino Pietropaolo[1], Fabrizio Murtas[2],
Antonella Scherillo[3], Anna Fedrigo[3], Frasncesco Grazzi[4]

1. *ENEA, Dipartimento di Fusione e Tecnologie per la Sicurezza Nucleare*
2. *STFC, ISIS Facility, UK*
3. *Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati*
4. *Consiglio Nazionale delle Ricerche, Istituto di Fisica Applicata*

The upgraded version of the GEM side-on thermal neutron detector was successfully tested in a neutron diffraction experiment on a reference sample using the INES diffractometer at the ISIS spallation neutron source, UK. The performance of the new $^{10}B_4C$ based detector is compared to that of a standard 3He tube, operating at the instrument as a part of the detectors assembly. The results show that the upgraded detector has a better resolution and an efficiency of the same order of magnitude of a ^3He-based detector.

Ice XVII: structural and dynamical properties of the new form of porous ice

Leonardo del Rosso[1], Milva Celli[1], Daniele Colognesi[1], Francesco Grazzi[1], Lorenzo Ulivi[1]

1. *CNR - Istituto di Fisica Applicata "Nello Carrara" Sesto Fiorentino, Italy*

Water exhibits several solid structures, depending on thermodynamic conditions. The latest-discovered crystalline form is ice XVII [1], which is obtained by the application of an annealing treatment to an H_2-filled ice sample in the C_0-phase [2] recovered at room pressure and 77 K. An impressive property of this new phase of water, which is metastable at ambient pressure and below 130 K, is its porosity, i.e. its capacity of adsorbing gas (e.g. H_2), even at a pressure well below 1 bar. For this reason, ice XVII represents an interesting system for the study of both fundamental aspects, related to the quantum behavior of the confined hydrogen molecules, and applicative ones, among which hydrogen storage is surely the most significant. In this talk we discuss the crystalline structure of D_2O ice XVII, that was resolved by means of neutron diffraction data taken on the OSIRIS instrument [3]. The dynamics of the adsorbed molecules (guests) inside ice XVII (host) has been investigated through high-resolution inelastic neutron scattering experiments performed on the TOSCA spectrometer and via molecular dynamics calculations [4]. The use of two different strong incoherent scatterers (H_2 and HD) as molecular guests of the deuterated host structure allowed to unequivocally assign the measured spectral bands to rotational and center-of-mass translational transitions, thus enabling to portray a picture of the confined motion of a hydrophobic guest in this novel inclusion compound.

[1] L. del Rosso, M. Celli, L. Ulivi, *Nat. Commun.* **7**, 13394 (2016).
[2] V. S. Efimchenko et al., *J. AlloysComp.***509**, S860 (2011).
[3] L. del Rosso et al., *J. Phys. Chem. C* **120**, 26955 (2016).
[4] L. del Rosso et al., *Phys. Rev. Mat.* **1**, 065602 (2017).

The analysis of some Indo-Persian daggers from the Wallace Collection at the Italian Neutron Experimental Station, ISIS, Didcot, and their results

David Edge, Alan Williams, Francesco Grazzi, Antonella Scherillo

A number of *katars* (Indo-Persian daggers) have been studies by TOF-ND on INES and yielded surprising results. Many were made in part out of *wootz* (patterned crucible steel) but also both iron and other steels were employed in construction, using mixed metals. The details of their construction will be presented. These are surprising and often counter-intuitive, and possible reasons for this will be discussed.

BRISP_X: a project for the upgrade of the BRISP spectrometer at the ILL

F. Formisano[1], A. De Francesco[1], A. Laloni[1], A. Cunsolo[2], E. Farhi[3], E. Guarini[4],
F. Sacchetti[5], and M. Zanatta[6]

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2. *Brookhaven National Laboratory (BNL), Upton NY, USA.*
3. *Institut Laue-Langevin (ILL), Grenoble, France*
4. *University Of Florence, Firenze, Italy,*
5. *University Of Perugia, Perugia, Italy*
6. *University Of Verona, Verona, Italy*

We will briefly retrace the technical and scientific history of BRISP, the Italian (CNR) and German (University of Marburg) spectrometer operating at the ILL since the end of 2007.
The scientific outputs of BRISP shows lights and shadows: despite the intrinsic difficulties of the neutron Brillouin technique, BRISP has yielded results not obtainable elsewhere, thus evidencing the need of a neutron spectrometer accessing the dynamics of condensed matter systems at small angles and thermal energies. However, the current position of the instrument results in an unfavourable signal-to-noise ratio that may strongly affect a proper extraction of the quantities of interest from the raw data.
We present here the status of BRISP_X, an upgrade project aiming at overcoming the BRISP limitations, and therefore offering to the scientific community an instrument able to perform neutron Brillouin scattering in a much extended family of materials.

Anisotropy of Co^{II} transferred to the Cr_7Co polymetallic cluster via strong exchange interactions

E. Garlatti[1,2], T. Guidi[1] A. Chiesa[2,3], S. Ansbro[4,5], M.L. Baker[6], J. Ollivier[5], H. Mutka[5], G.A. Timco[4], I. Vitorica-Yrezabal[4], E. Pavarini[3,7], P. Santini[2], G. Amoretti[2], R.E.P. Winpenny[4], S. Carretta[2]

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The Cr_7Co ring represents a model system to understand how the anisotropy of a Co^{II} ion is transferred to the effective anisotropy of a polymetallic cluster by strong exchange interactions [1]. By combining EPR and INS measurements with spin Hamiltonian and ab initio calculations, we have been able to investigate in detail the anisotropy of the Co^{II} ion embedded in the antiferromagnetic (AF) ring. Indeed, since the ring is isostructural with the other previously studied Cr_7M AF rings, we have been able to focus on Co^{II} single-ion anisotropy and on Cr-Co exchange interactions. Our results demonstrate a strong and highly anisotropic exchange interaction between Co^{II} and the neighbouring Cr ions, which effectively transmits the anisotropy of Co^{II} to the whole molecule. This study is a starting point for the design of new systems, where high-spin ions are strongly coupled to a few very-anisotropic ions like Co^{II}. Indeed, these systems represent a promising route for reaching the strong-coupling between single molecules and photons in coplanar superconducting resonators and building scalable quantum information architectures.

[1] E. Garlatti, T. Guidi, A. Chiesa, S. Ansbro, M.L. Baker, J. Ollivier, H. Mutka, G.A. Timco, I. Vitorica-Yrezabal, E. Pavarini, P. Santini, G. Amoretti, R.E.P. Winpenny, S. Carretta, Chem. Sci. **9**, 3555-3562 (2018).

Modelling Option USANS upgrade: the project OPUS for LoKI@ESS and the upgrade of D11@ILL

Claudia Mondelli [1], Víctor M. Galván Josa [1], Emmanuel Farhi[2], Ralf Schweins[2] and Andrew Jackson[3]

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2. *Institut Laue - Langevin, 71 Avenue des Martyrs, Grenoble, 38000, France*
3. *European Spallation Source, PO Box 176, Lund, 221 00, Sweden*

One of current challenges in soft matter and materials science involves understanding complex systems with high hierarchical order on a manifold length scale. SANS is one of the well established techniques for that purpose, and recently, it further expanded its capabilities by USANS.

OPUS (OPtion USans) is a project dedicated to study an USANS option for the ESS (European Spallation Source) ToF-SANS instruments LoKI and SKADI. The basis of our approach is the Small Angle Multi Beam Analysis proposed by Roland Gähler[1]. The fundamental idea is to multiplex the scattering experiment in order to achieve a gain in intensity over an equivalent single pinhole geometry.

We performed McStas simulations in order to project and design a specific optics to adapt the original approach to the characteristics of LoKI and SKADI instruments at ESS: addition of two multi-hole grids, multi lenses and a high resolution detector. Furthermore we extended this ray tracing study to the USANS prototype, based on the same principle, designed for the upgrade of D11 at ILL.

We present here the conclusive results of the McStas-simulated virtual experiments using virtual samples -spheres and cylinders- for both instruments. The effects of set up misalignments, wavelength spread and detector resolution on the ultimate intensity and resolution are also studied.

[1] R. Gähler *et al.* Proc. SPIE 4785; Advances in Neutron Scattering Instrumentation; Ed: Anderson I., Guerard B. (2002) 153.

Neutron scattering for sustainable energy materials: investigations of proton dynamics in acceptor-doped barium zirconates

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3. *Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Göteborg, Sweden*

Proton conducting oxides are currently receiving considerable attention for their use as electrolytes in solid oxide fuel cells. One of the main challenges for these devices is to combine the advantages of a solid electrolyte with those of operational temperatures below 750 ºC, which is at present hampered by insufficient conductivities in the targeted *T*-range. The development of new electrolytes meeting the requirements for applications depends on a better understanding of the proton conduction mechanism. To this aim, systematic QENS investigations over a wide *Q*-*E* range were conducted on hydrated acceptor-doped barium zirconates, with focus onto the effect of the type and concentration of dopant atoms on the atomic-scale proton dynamics.

The results show complex dynamics, arising from a distribution of different proton sites. At ps time scale, localized displacements interpretable as proton jumps and reorientations of the hydroxyl groups are disclosed. Faster local motions are observed for the more distorted structures associated with higher doping levels. The analysis of the dynamics at longer time scales reveals long-range proton diffusion which can be described as a Chudley-Elliot jump-diffusion process. Higher doping concentrations lead to higher activation energies, but larger fractions of mobile protons. This new insight can be useful for the design of improved proton conductors for technological applications.

Neutron reflectivity of layers formed by nanoparticle-surfactant complexes at the oil/water interface

Davide Orsi[1], Libero Liggieri[2], Sara Llamas[2], Francesca Ravera[2], Eva Santini[2], Mario Campana[3], Luigi Cristofolini[1,2]

1. *Dept. of Mathematical, Physical and Computer Sciences, University of Parma, Italy.*
2. *CNR – Inst. for Condensed Matter Chemistry and Energy Technologies, Genoa, Italy.*
3. *STFC Rutherford Appleton Labs - Harwell Oxford, Didcot, United Kingdom.*

Pickering emulsions, i.e. emulsions stabilized by solid particles, are important in many food, cosmetic and pharmaceutical applications. Even if they have been known for more than a century, they still pose important challenges to the researchers.

We report on a neutron reflectivity (NR) study of the layers formed by amphiphilic complexes of silica nanoparticles (NP) and cationic surfactant CTAB at the oil (dodecane)-water interface. Dilational rheology and interfacial tensiometry provided a general understanding of NP-surfactant layers at liquid interfaces [1], but have also evidenced a complex interplay between the components. In particular, it is still unclear if reorganizations of surfactant-NP complexes and/or a redistribution of the surfactant between the complexes and the free liquid interface may occur at the interface[1,2].

To elucidate these aspects, we employed for the first time NR [3] to study these complexes at the interface. Experiments were performed on INTER (ISIS, Rutherford Appleton Labs) on a set of different contrast matched sample. We investigated the mixed layer structure and the redistribution of surfactant between the different interfaces: particle/oil, particle/water, water/oil. Accurate modelling of the data allows to estimate the contact angle, an important parameter in determining the stability of Pickering emulsions. We find evidence of an oil/water emulsion layer at the interface. Results are discussed in the light of previous findings.

[1] F. Ravera *et al.*, J. Phys. Chem. B **110**, 19543 (2006).
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On the slowing down of 14 MeV fusion neutrons: a spectrometry benchmark and future perspectives

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The spectral fluence rate of the thermalized neutron field obtained by slowing down the 14 MeV fusion neutrons produced at the accelerator-driven Frascati Neutron Generator is measured by means of the Bonner Sphere Spectrometer. Neutron thermalization is achieved by means of a moderator assembly made of a Copper pre-moderator and a polyethylene moderator. A Monte Carlo simulation reproducing the experimental set up is also performed by means of the MCNP code and the results compared to the experimental data. The benchmarked Monte Carlo is then used to predict the brilliance of a H_2O (thermal) and liquid D_2 (cold) moderator operating at a potential high intensity 14 MeV neutron continuous source featuring a neutron emission rate of 10^{15} s^{-1}. Eventually, the moderators brilliance predicted by the model is compared to that of the liquid H_2O and D_2 moderators operating at the SINQ continuous spallation neutron source. The results obtained show that if a D-T neutron source featuring a continuous neutron emission rate of 10^{15} s^{-1} could be made operative, it could be effectively exploited for neutron science as the neuron spectrum provided by the conceived moderators and their brilliance are similar to those presently achieved at a continuous spallation neutron source such as SINQ.

Hydrogen Bond Length as a Key to Understanding Sweetness

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Neutron diffraction experiments have been performed to investigate and compare the structure of the hydration shell of three monosaccharides, namely fructose, glucose and mannose. It is found that, in spite of their differences with respect to many thermodynamical quantities, bio-protective properties against environmental stresses and taste; the influence of these monosaccharides on the bulk water solvent structure is virtually identical. Conversely, these sugars interact with the neighboring water molecules by forming H-bonds of different length and strength. Interestingly, the sweetness of these monosaccharides, along with that of the disaccharide trehalose, is correlated with the length of these H-bonds. This suggests that the small differences in stereochemistry between the different sugars determine a relevant change in polarity, which has a fundamental impact on the behavior of these molecules *in vivo*. Finally, we notice that the almost negligible, yet similar, perturbation brought by the investigated carbohydrates to the tetrahedral structure of water cannot be taken as a key to explain the differences in terms of bio-protection (both against dehydration and temperature stress) and glass transition temperatures observed for the solutes. In particular, as far as the bio-protection mechanism is concerned, the hypotheses that carbohydrates act as water substitutes or by segregating water at the surface of a proteinare better supported by our data.

Neutron and synchrotron-based techniques for material science

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Science of matter requires the capability to understand he intimate relationships between the microstructure and the macroscopic properties of materials. A successful approach to investigate complex problems in material science is constituted by the joint use of multiple complementary experimental techniques, each of which is able to gives us a small piece of the same puzzle. Neutron scattering techniques are an indispensable tool for studying atomic structure and dynamics in condensed matter because of their unique properties but the information achieved by neutron experiments can be considerably enhanced and complemented by other techniques, based on different physical processes. In this contribution, we will present some examples where the joint combination of neutron and synchrotron-based techniques is used for addressing a large arrays of open issues in material science, especially for researchers interested in biological problems.

Hydrogen dynamics in complex borohydrides

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Quasielastic neutron scattering was used to investigate the (sub-)picosecond timescale hydrogen dynamics of the complex borohydrides $Mg(BH_4)_2$ in the a- and b-modifications, $LiBH_4$ in the low and high temperature crystal structure, and the 1:1 molar mixture of $LiBH_4$+a-$Mg(BH_4)_2$. All investigated compounds show a rich dynamic behavior below an energy range of $\Delta E = 10$ meV with the superposition of rotational dynamics of the constituent $[BH4]^-$ anions and low lying lattice modes. For $Mg(BH_4)_2$, the rotational diffusion of the $[BH_4]$ units was found to be much more activated in the metastable b-polymorph compared to the a-phase, and the low lying lattice modes are even softer in the former crystal structure. In $Mg(BH_4)_2$, the structural phase transition is mainly governed by the lattice dynamics, while alkaline LiBH4 exhibits a transition of the $[BH_4]$ rotations around the phase transition temperature. Ball milled $LiBH_4$ + a-$Mg(BH_4)_2$ remains a physical mixture of the parent compounds and each component retains its characteristic dynamic signature up to the melting temperature.

Physico-chemical insights into Cardiolipin-containing Lipid Bilayers

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Cardiolipin (CL) lipids are a group of anionic phospholipids composed of two phosphate moieties, each attached to two hydrocarbon chains *via* a glycerol backbone. CL is present in the inner membrane of Gram-negative and Gram-positive bacteria as well as in the mitochondrial and chloroplast inner membranes of eukaryotes [1]. Two phosphatidic acid moieties connect with a glycerol backbone in the center to form a dimeric structure, with four acyl chains and potentially two negative charges. The four acyl chains in cardiolipin give this lipid molecule species particular properties. However, the function of cardiolipin (CL) is not well understood in the context of dynamic membrane assembly as well as the resulting membrane structure [2].

This study is aimed to investigate the cardiolipin influence on the physico-chemical properties, such as mesoscopic and microstructural organization of lipid vesicles formed by zwitterionic (1-palmitoyl-2-oleoyl phosphatidylethanolamine, POPE) and anionic (1-palmitoyl-2-oleoyl-sn-glycero-3-[phospho-rac-(1-glycerol)], POPG) lipids, and cholesterol. Two different composition of cardiolipin are investigated, also in the absence and presence of Ca^{2+} ions. In this way, neutron scattering experiments permit to clearly define the role of cardiolipin, in terms of its headgroup and acyl chains regions, in modulating the phospholipids organization in the presence of cholesterol into lipid bilayers.

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Neutron techniques and the study of arms and armour

Alan Williams, Francesco Grazzi, David Edge, Antonella Scherillo, Nikolai Kardjilov

While excavated swords can generally be sampled for metallography, this is ruled out for museum objects. For the study of swords and armour, non-invasive techniques are essential. We have found that neutron diffraction, carried out on INES (Italian Neutron Experimental Station) at ISIS, has been most valuable.

The Wallace Collection is a national museum in London which possess the largest collection of princely European Armour in London, and one of the most important collections of Oriental Arms and Armour outside the subcontinent. As part of the cataloguing project for the latter, many of the 2000+ objects have been cleaned and photographed, and 48 (up to now) have been examined by phase-analysis using neutron diffraction at INES. These results will be discussed.

Patterns in *wootz* ("Damascus steel") can be identified in many overpolished blades, and the different methods of their formation are being studied. Because of the value of such blades, methods of contemporary counterfeiting can be discovered. The novel constructional techniques used in Indian *katars* (daggers) have been investigated for the first time.

European helmets from this, and other museums, have also been analysed on INES, as well as being the subjects of phase-contrast image analysis on CONRAD at the Helmholtz Zentrum, Berlin, which is proving to be a viable technique for revealing armourers' marks which have become obscured over time.

Clip talks

Neutron scattering on gelatin: relevance for analog modelling

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Gelatin is one of the most versatile biopolymers that founds widespread use in food, pharmaceutical and cosmetic industries, among others. Besides these common applications, gelatin has proved to be particularly useful in analog modeling: a lab discipline that allows simulating in a convenient spatio-temporal scale geological processes that would not be possible to observe otherwise due to the multi-century timing. One of the biggest challenges for analog modellers is the selection and calibration of materials with specific rheology to ensure the rheological similarity with the natural prototype. While rheological behavior of gelatin under different experimental conditions can be easily characterized with rheometric measurements, the relationship between gel microstructure and rheology can only be guessed. However, understanding how modifications to the gel network relate to rheological properties would have important implications on designing new analog materials with complex, hence realistic, behavior. Here, we seek to promote discussion about the use of neutron scattering for experimental tectonics applications. This will allow broadening our knowledge on gels and other materials commonly adopted to simulate the dynamics of our planet, while potentially opening new fields of applications for this technique.

Trehalose Protectant Activity for peptide hydration

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The interactions of carbohydrates with biomolecules are of great interest, as these interactions are responsible for their protection against environmental stresses. Among the different bioprotectants, the disaccharide trehalose is undoubtedly the best performer. To date there are three possible hypotheses that try to explain structural and dynamical mechanisms of bioprotective features. The first is the substitution, in which the trehalose replaces the water molecules of the first hydration shell, maintaining peptide structure and functionality [1,2]. The second is the vitrification, where trehalose interacts with water and the system undergoes a glass-like stabilizing transition [3,4]. The third is the confinement, where a few water molecules mediate the peptide-sugar interaction and trehalose creates a cage around the hydrated molecules [5]. To clarify which of these hypotheses better describes the real situation, a series of neutron diffraction with H/D isotopic substitution experiments, combined with EPSR computer simulations, have been performed. The obtained results highlight that the addition of trehalose in solution does not alter the peptide first hydration shell and that trehalose forms a protective cage around the hydrated peptide. Therefore, this data do not sustain the substitution hypothesis. Further studies are required to investigate if bio-protection is due to vitrification or confinement.

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Short-time self-diffusion of immunoglobulin under different crowding conditions

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Tra il 10 e il 40% dei fluidi intra ed extracellulari degli organismi viventi è occupato da macromolecole quali proteine, il cui principale processo di trasporto passivo è la diffusione. Tali condizioni ad elevate concentrazioni di macromolecole vengono dette di "affollamento macromolecolare" e possono influire su velocità di reazione, stabilità termica e diffusione delle proteine [1]. Qui presentiamo uno studio di retrodiffusione neutronica (neutron backscattering) riguardante la diffusione su scale di tempo di alcuni nanosecondi di immunoglobuline (Ig), proteine con la funzione di anticorpi, in soluzioni acquose. Consideriamo due sistemi: Ig e seralbumine (i due tipi di proteina più abbondanti nel siero sanguigno) e Ig in lisato cellulare, che mima l'ambiente cellulare.
Per studiare gli effetti dell'affollamento macromolecolare sulla dinamica di Ig in ambienti differenti variamo sistematicamente la concentrazione di Ig, seralbumina e lisato, nei rispettivi sistemi. Nonostante la diversità di questi ambienti, la diffusione di Ig (in alcuni nanosecondi) in funzione della frazione di volume totale del sistema è in buon accordo con quella di Ig in pura D2O, in funzione della sua stessa frazione di volume [2], il che è indice di un ruolo cruciale delle interazioni idrodinamiche anche in ambienti complessi, simili a quelli biologici.

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Magnetic Exchange and Crystal Field excitations of asymmetric Lanthanide dimers: An INS insight

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Molecular nanomagnets (MNMs) with lanthanide 4f ions core exhibit slow relaxation of magnetization at (relatively) high temperatures, and large single-ion anisotropies rendering them interesting for quantum information processing (QIP) and dense information storage (DIS) applications. However, their crystal field (CF) structure and relaxation dynamics are difficult to interpret, because of the large number of terms in Hamiltonian and scarcity of available experimental data. Understanding Ln-Ln interactions and a transferrable microscopic Hamiltonian is therefore of utmost importance in 4f MNMs for exploiting their potential for applications.

We performed Inelastic neutron scattering (INS) measurements, aided by EPR, FIR, and CASSCF-SO calculations to elucidate crystal-field and magnetic interactions within the asymmetric dimetallic compounds $[hqH_2][Ln_2(hq)_4(NO_3)_3]\cdot MeOH$, (Ln = Er(III), Yb(III), Dy(III); hq = 8-hydroxyquinoline)[1]. High-energy INS experiments using MARI spectrometer enabled us to detect single-ion CF excitations. Whereas exploiting high-resolution IRIS and LET spectrometers we detected the splitting of dimer ground manifold due to the Ln-Ln interaction. Using these results, we individually determined the local electronic structure of inequivalent sites. At last, we show that the dipolar interactions are a significant component of the magnetic interactions in Er_2 and Dy_2, while for Yb_2 super-exchange interactions are important and the dipolar exchange is marginal.

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The effects of manufacturing processes on historical ceramic morphology studied by Small Angle Neutron Scattering

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Ralf Schweins[3], and Elti Cattaruzza[2]

1. *CNR-IOM-OGG, Institut Laue - Langevin, 71 Avenue des Martyrs, Grenoble, 38000, France*
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Analytical techniques applied to art and archaeology objects can give the opportunity of gaining information about their composition and, therefore, to answer questions regarding where, when or by whom such artefacts were made. Additionally, these studies can help us to understand the manufacturing processes and technology, providing clues for interpreting the social, political, economic and cultural context of the civilizations involved. Such investigations are also valuable and, in some cases, fundamental for conservation, restoration and authentication projects [1]. In this work, we present a SANS study performed on historical ceramics fragments, in order to correlate the characteristics (total volume and pore dimensions) of the ceramics found in several German and Italian sites with specific production techniques. SANS measurements of samples immersed in heavy water were also performed to investigate the role of closed porosity on the material structure, its behaviour/evolution during the firing process and its effects on the mechanical properties. Laboratory-made samples with different clays and firing conditions were also characterized in order to compare them with the ancient ceramics.

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Posters

Probing Structure and Mobility of Proteins in the Amorphous State at Low Hydration

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3. *Department of Materials, University of Oxford, Parks Road, Oxford, UK*

The characterization of proteins in the dry state has implications for the pharmaceutical industry, since it provides deeper understanding of the effect of lyophilisation on the stability and biological activity of bio-macromolecular drugs. We have performed structural and dynamical analyses on a series of lyophilised and hydrated bio-macromolecules with varying degrees of structural complexity by means of Molecular Dynamics (MD) simulations; the simulated dynamical results being compared to experimental findings obtained from neutron scattering.

Atomistic simulation of lyophilised proteins is still a challenge since the available force fields, and water molecule topology, used for the modelling have to be carefully correlated with experiment. Fortunately, the outputs from MD simulations, and the time and length scales probed, align directly with those accessed by neutron scattering. In particular, the method of Quasi-Elastic Neutron Scattering (QENS) can explore picosecond to nanosecond dynamics of macromolecular species and thus help validate the efficacy of the MD protocols applied.

Here we report on the simulated effect of temperature and hydration on the structural features of the proteins, focusing particularly on the predicted changes in secondary structure and radial distribution. We also present a comparison of the temperature dependence of the mean squared displacement parameter, obtained by analysing the MD trajectories, with those resulting from QENS measurements.

The analysis of some Indo-Persian daggers from the Wallace Collection at the Italian Neutron Experimental Station, ISIS, Didcot, and their results

David Edge, Alan Williams, Francesco Grazzi, Antonella Scherillo

A number of *katars* (Indo-Persian daggers) have been studies by TOF-ND on INES and yielded surprising results. Many were made in part out of *wootz* (patterned crucible steel) but also both iron and other steels were employed in construction, using mixed metals. The details of their construction will be presented. These are surprising and often counter-intuitive, and possible reasons for this will be discussed.

In-situ gas-sorption neutron studies at ISIS

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The use of *in situ* techniques with neutrons is often complicated by the duration of data acquisition and the availability of specific sample environment at the neutron facility. When dangerous gases (such as hydrogen or ammonia) are being used, particular efforts are needed in order to meet safety regulations and experimental requirements.

Over the last 2 years an effort has been pursued at ISIS to design and develop *in situ* gas storage capabilities in order to carry out experiments on both diffraction and spectroscopy beamlines. In this work we discuss the use of a new available sample environment that allow to investigate hydrogen storage materials by means of H_2 (and D_2) gas sorption cycling at pressures and temperatures relevant for industrial applications (0-200 bar and 77-673 K) on neutron instruments. A full control over the pressure is achieved through the use of a smart automatic pressure controller scripted and monitored from a computer. A small amount of sample (0.5-1.5 cm^3) is required thanks to the design of special high-pressure cells.

The high neutron flux available on WISH is optimal to detect structural changes occurring in the range of seconds. For this reason, the commissioning of this new setup was carried out on this beamline on a novel class of hydrogen storage materials (intercalated fullerides) and allowed a full structural study upon multiple-absorption/desorption cycles. The same setup is designed to be used successfully on spectroscopy beamlines such as TOSCA, IRIS, OSIRIS, and MAPS, as well as for tomography studies (i.e. IMAT).

Upgrades at the high-resolution backscattering spectrometer SPHERES

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1. *Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Garching, Germany*

The SPectrometer for High Energy RESolution (SPHERES) at MLZ is a third generation backscattering spectrometer with focusing optics and phase-space transform (PST) chopper. SPHERES enables the investigation of dynamics in a range of ± 31 μeV with a high energy resolution of about 0.65 μeV. Typical applications cover several diverse fields such as hyperfine splitting in magnetic materials, H-diffusion in ionic conductors, relaxation processes in glasses, rotational tunneling of molecular rotors, dynamics in complex materials such as polymers or biological systems.

Different components of the instrument have been upgraded to further improve the instrument performance. A new, more compact, one-wing PST chopper was installed some recent years ago. The new device can be operated close to the optimum velocity for the phase-space transformation and has graphite deflector crystals with higher reflectivity and mosaicity. As a result, the intensity in most detectors is doubled. More recently the focusing neutron guide was replaced with an elliptic guide, optimized based on simulations. With the new elliptic guide another intensity gain at the sample position of about 30% was obtained. Together with this upgrade, also a new background chopper was installed about 2m upstream of the PST chopper, to further reduce background. This will then also allow for a high signal-to-noise setup by eliminating every second pulse, albeit at the cost of intensity.

Role of native oxide layer in silicon anodes for Li/S

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Lithium/sulfur (Li/S) and Lithium/air systems are possible candidates for future electrochemical energy storage, due to higher gravimetric density compared to conventional Li-ion batteries. In these systems, a lithiated silicon (Si) electrode often replaces the Li metal anode, used as a Li ions reservoir. Detailed studies on lithiation and delithiation of Si anodes are of fundamental importance in understanding capacity fading effects. Silicon crystals are used with the native silicon dioxide (SiO2) layer: upon lithiation and delithiation, Li ions interact first with the SiO2, and subsequently intercalate in the Si crystal forming a Li/Si alloy. Due to the negative scattering length density of Li, neutron reflectometry is a powerful technique for investigating lithiation and delithiation of Si anodes. Two different Li/Si cells were prepared, one with and one without native oxide layer (removed using HF etching) on the Si anode. Both were measured at the reflectometer V6 at the BER II neutron source, to shade some light on the role of the SiO2 native layer formation and its (ir-)reversibility using both electrochemical (CV, EIS, charge/discharge) and in situ/operando neutron reflectometry measurements.

Neutron techniques and the study of arms and armour

Alan Williams, Francesco Grazzi, David Edge, Antonella Scherillo, Nikolai Kardjilov

While excavated swords can generally be sampled for metallography, this is ruled out for museum objects. For the study of swords and armour, non-invasive techniques are essential. We have found that neutron diffraction, carried out on INES (Italian Neutron Experimental Station) at ISIS, has been most valuable.

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Indice


SISN