SISN

Società Italiana di Spettroscopia Neutronica

Congresso Annuale

13-14 Settembre **2007**

Sestri Levante

Programma & Abstracts

Ho scoperto le barche che molleggiano
Sole, e le osservo non so dove, solo.

Congresso Annuale 13-14 Settembre **2007**
Sestri Levante

Programma

Giovedì 13 Settembre 2007

8.45 – 9.00	Introduzione e benvenuto	
9.00 – 10.00	S. Carretta	"Spin dynamics in magnetic molecules probed by inelastic neutron scattering"
10.00 – 11.00	J. Teixeira	"Study of the dynamics of hydrogen bonds in water and consequences for the unusual behavior of supercooled water"
11.00 – 11.20	*Coffee break*	
11.20 – 11.45	L. Capogna	"High pressure studies of the magnetic phase diagram of $La_{0.75}Ca_{0.25}Mn\ O_3$ and $La\ Mn_{0.7}Ga_{0.3}O_3$"
11.45 – 12.10	L. Ulivi	"Quantum rattling motion of hydrogen molecules in clathrate hydrate"
12.10 – 12.35	S. Capponi	"Structure and dynamics of PVME. A neutron scattering and molecular dynamics simulation study"
12.35 – 13.00	G. Venturi	"Determinations of $S(Q,\omega)$ of liquid CD_4 revealing the molecular arrengement and the role of anisotropic interactions"
13.00 – 14.30	*Pranzo*	
14.30 – 15.45	**Sessione Poster**	
15.45 – 16.10	E. Cornicchi	"Studio comparativo della dinamica veloce di lisozima e DNA e ruolo dell'environment"
16.10 – 16.35	R. Sinibaldi	"Detailing the solvation layer composition of proteins in mixed solutions: a SANS study"
16.35 – 17.00	*Coffee break*	
17.00 – 19.30	**Assemblea SISN**	
20.30	*Cena e, a seguire,*	**premiazione Poster e Relazioni di giovani ricercatori**

Venerdì 14 Settembre 2007

9.00 – 10.00	G. Artioli	"Neutrons in archaeometry"
10.00 – 11.00	L. Cantù	"Neutrons for biological soft matter"
11.00 – 11.20	*Coffee break*	
11.20 – 11.45	A. Paciaroni	"Studying the low-frequency vibrational features of water at the interface with a deuterated protein"
11.45 – 12.10	A. De Francesco	"A new physical approach to understanding demyelization: investigation of the structure and dynamics of model myelin sheaths"
12.10 – 12.35	M. Zoppi	"Microscopic structure of single walled nanotubes and allotropic impurities"

Sessione Poster

Giovedì 13 Settembre 14.30 – 15.45

U. Bafile , F. Barocchi , E. Guarini , M. Sampoli, G. Venturi
"Large wave vectors sound excitations in the collective dynamics of fluids"

F. Grazzi, L. Bartoli, **M. Celli**, S. Imberti, M. Zoppi
"*The Italian Neutron Experimental Station (INES) at ISIS: status and development"*

C. Chiapponi, M.T. Di Bari, A. Deriu, F. Sonvico, P. Santi, S. Nicoli, C. Padula, J. Ollivier
"*Water diffusiviity in PVA-based transdermal patches*"

R. Favillini, U. Bafile, F. Barocchi , F. Formisano, E. Guarini, A. Orecchini, M. Sampoli, G. Venturi
"Neutron scattering determination of the dynamic structure factor of liquid CO_2*"*

Y. Gerelli, MT Di Bari, A. Deriu, F. Sonvico, C. Como, P. Colombo
"*Neutron investigation of the structure and organization of phospholipid/saccharide nanoparticles*"

F. Rustichelli, F. Fiori, C. Renghini, **E. Girardin**, G. Albertini, K. Konopka
"Small Angle Neutron Scattering characterisation of Al_2O_3*/Ni-P nanocomposites"*

R. Magli, S. Bianchi, G. Andrè, M. Benvenuti, P. Costagliola
"Etruscan weapons investigated through neutron radiography and diffraction"

M. G. Ortore, R. Sinibaldi, F. Spinozzi, P. Mariani
"Combined SANS/SAXS study of the BSA solvation layer in urea aqueous solutions"

M. Plazanet, S. Eibl, H. Schober
"*Dynamics in an ultra fragile glass former: Decalin"*

S. Dante, A. Relini, S. Torrassa, T. Hauss, M. Bucciantini, M. Stefani, A. Gliozzi, **R. Rolandi**
"*Interaction between amyloid aggregates and phospholipid membranes: a neutron diffraction study*"

Congresso Annuale 13-14 Settembre **2007**
Sestri Levante

Il comitato ringrazia gli sponsor che, in varie forme, hanno permesso l'organizzazione del congresso SISN 2007.
Si ringraziano in particolare

Centro di Ricerca e Sviluppo *SOFT* del CNR-INFM
(Consiglio Nazionale delle Ricerche – Istituto Nazionale per la Fisica della Materia)

e

CNISM
(Consorzio Nazionale Interuniversitario per le Scienze fisiche della Materia)

La giunta SISN e i direttori delle Giornate Didattiche SISN 2007 ringraziano inoltre l' **Institut Laue-Langevin** (ILL) *di Grenoble per la collaborazione e disponibilità all'organizzazione delle sessioni sperimentali per gli studenti.*

Abstracts

Relazioni ad invito

Spin dynamics in magnetic molecules probed by inelastic neutron scattering

Stefano Carretta[1]

[1] *Dipartimento di Fisica, Università di Parma, Italy*

Magnetic molecules are one of the best examples of ensemble of noninteracting quantum objects embedded in a solid-state environment. Of particular relevance are molecules containing transition-metal ions whose spins are so strongly exchange coupled that at low temperature each molecule behaves like a single-domain particle with fixed total spin S. Two major advantages in the research on these systems are on one side the outstanding degree of accuracy by which their magnetic dynamics can usually be modelled, and on the other side the opportunity to chemically engineer molecules possessing desired physical properties. Besides having obvious fundamental interest, the comprehension and control of the dynamics of these systems is necessary for implementing the envisaged technological applications as nanoscopic classical or quantum bits. The crucial step to reach a deep understanding of the magnetic dynamics of these molecules is the determination of the molecular eigenstates and eigenvalues.
In this talk, I will show that inelastic neutron scattering (INS) is the most powerful technique to investigate the molecular spin dynamics over different timescales. Some recent results on different families of magnetic molecules will be briefly reviewed. In particular, I will concentrate on the possibility to investigate by INS quantum coherent phenomena like Quantum Oscillations of the Total Spin or the potential exploitation of these systems for Quantum Information Processing.

Study of the dynamics of hydrogen bonds in water and consequences for the unusual behaviour of supercooled water

Josè Teixeira and Stéphane Longeville [1]

[1] *Laboratoire Léon Brillouin, CEA/Saclay, 91191 Gif-sur-Yvette, France*

Since more than 30 years the puzzle of supercooled water remains object of debate. The more recent developments have been achieved almost exclusively by computer simulations of the molecular dynamics using different "effective" potentials. Some of them demonstrate the existence of liquid-liquid phase transitions and of a critical point under temperature-pressure conditions not accessible to real experiments. It is not obvious that such results apply to supercooled water.
We use coherent quasi-elastic neutron scattering in an original way that partly discriminates the dynamics of different partial components of the scattering law. The results confirm that the dynamics of hydrogen bonds follows an Arrhenius behaviour. We argue that the dynamics of supercooled water between the homogeneous nucleation temperature (not accessible to simulations) and the glass transition is determined by the dynamics of the bonds similarly to beta relaxation in polymer melts.

Neutrons in archaeometry

Gilberto Artioli[1]

[1] *Dipartimento di Geoscienze, Università di Padova, Italy*

Neutron probes are primary sources for the non-invasive characterization of materials related to cultural heritage. Their employment in the investigation of archaeological objects and art works encompasses imaging, chemical analysis, and crystallographic analysis, including phase identification, texture analysis, and structure and microstructure analysis. In principle, many of these information may be obtained simultaneously in a single combined experiment, thus minimizing neutron exposure and the risks and the costs related to object's handling.
As a successful example, diffraction based crystallographic texture analysis (CTA) has been recently applied to the investigation of archaeological metals. When performed using penetrating probes and adequate detector coverage of reciprocal space, for example using large detector arrays and/or ToF mode, CTA allows simultaneous identification and quantification of crystalline phases, besides the microstructural and textural characterization of the object. CTA can therefore be effectively used as a totally non invasive tool for metallographic analysis, thus proving to be a powerful tool for the interpretation of ancient metal working techniques. Fig. 1 shows an Aeneolithic copper axe from Montecchio Emilia, Italy, and Fig. 2 the pole figures reconstructed from neutron ToF diffraction data collected on the the axe at GEM instrument at ISIS.

Fig. 1. Aeneolithic copper axe from Montecchio Emilia, Italy now in the Museo Archeologico di reggio Emilia.

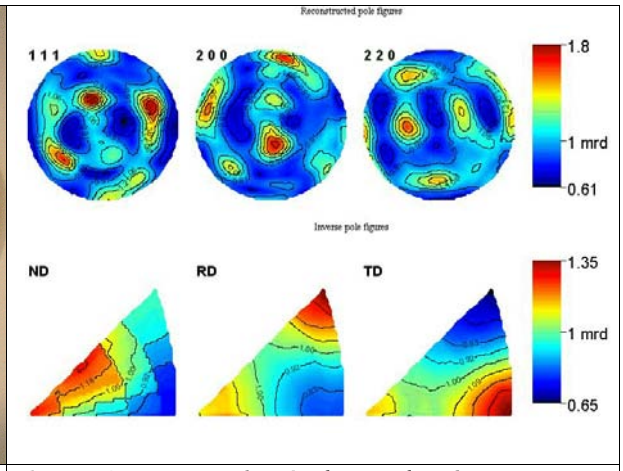


Fig. 2. Reconstructed pole figures for the copper axe obtained from ToF neutron diffraction data collected at GEM.

Neutrons for biological soft matter

Laura Cantù[1]

[1] *Dipartimento Chimica, Biochimica e Biotecnologie per la Medicina, Università di Milano, Italy*

Gangliosides are anionic glycosphingolipids, naturally occurring in the outer leaflet of plasma membranes, where they participate in lipid-driven microdomains. The tendency to cluster with respect to some other admixed lipids seems to be preserved also in simple biomimetic membranes, affecting their structural and dynamic properties in a non-trivial fashion, depending on their spatial distribution [1,2]. Moreover, ganglioside assemblies display coupled collective behaviours taking place both in their hydrophobic and hydrophilic regions [3,4]. This observation tributes to their structure/dynamics behaviour a putative biofunctional significance, with the intervention of one, or more, regulatory factor. Nonetheless, the extension and persistence of lipid-driven microdomains containing gangliosides is controversial. A direct observation in "unperturbed" disperse systems is still lacking. During the last years we have tried to apply neutron spectroscopy techniques to gain deeper structure/dynamics insight in simple biomimetic systems containing gangliosides. Often we used SANS on aqueous solutions of pure and mixed systems, sometimes employing partially deuterated admixed phospholipids, sometimes QENS [5] and also the neutron backscattering technique on oriented lamellar stacks [6]. We also applied neutron diffraction and reflection on lamellar stacks and a trial has been performed with the floating bilayer configuration. Few measurements with WANS have also been tried. Neutron spectroscopy experiments have often been paralleled by their X-ray counterpart, to profit from their complementary information and to overcome the difficulty of gangliosides deuteration by exploiting the different characteristics of neutron and X-ray contrast profiles. The obtained results support the concept of uneven distribution of gangliosides, depending on the system where they are embedded, with a pronounced influence on their environment.

[1] L. Cantù *et al.*, *Chem. Phys. Lipids* **55**, 223 (1990).
[2] P. Brocca *et al.*, *Langmuir* **20** (6), 2141 (2004).
[3] L. Cantù *et al.*, *Langmuir* **15** 4975 (1999).
[4] P. Brocca *et al.*, *Langmuir* (in press).
[5] P. Brocca *et al.*, *PhysicaB* **350**, e619 (2004).
[6] C. Caronna *et al.*, ICNS2005.

Congresso Annuale 13-14 Settembre 2007
Sestri Levante

Relazioni

High pressure studies of the magnetic phase diagram of $La_{0.75}Ca_{0.25}MnO_3$ and $La\,Mn_{0.7}Ga_{0.3}O_3$

M. Baldini[(1)], **L. Capogna**[(2)], E. Arcangeletti[(1)], I. Goncharenko[(3)], P. Postorino[(1)]

[(1)] *Dipartimento di Fisica, Università La Sapienza P.le A. Moro, 00185 Roma, Italy*
[(2)] *INFM CNR-SOFT, OGG 6 Rue J. Horowitz, 38042 Grenoble, France*
[(3)] *Laboratoire Léon Brillouin, CEA/Saclay 91191 Gif-sur-Yvette cedex Paris, France*

We have investigated the effect of high pressure on the magnetic structure of the prototypical colossal magnetoresistive manganite (CMR) $La_{0.75}Ca_{0.25}MnO_3$ and of a Ga^{+3} doped manganite $LaMn_{0.7}Ga_{0.3}O_3$ using neutron powder diffraction. Rare-earth manganites $A_{1-x}A'_xMnO_3$, (where A is a trivalent rare earth and A' a divalent alkali earth) exhibit Colossal Magneto-Resistance (CMR) in the doping range $0.2<x<0.5$. Double-Exchange (DE) qualitatively accounts for the closely related phenomena of CMR and temperature-driven transition from the paramagnetic insulating phase (high-temperature) to the ferromagnetic metallic one (lowtemperature). However the Jahn-Teller (JT) effect, i.e. the spontaneous distortion of the MnO_6 octahedron, competes with the delocalizing DE mechanism. Indeed JT is naturally associated with a sizeable electron-phonon coupling, which reduces the electron mobility. A complete description of the manganite properties at a microscopic level is further complicated by the presence of an antiferromagnetic (AF) Super-Exchange (SE) interaction between the S=3/2 spins of the localized t_{2g} electrons. AF-SE is relevant in the electron-doped regime ($x>0.5$) but could play a role also in the CMR region.

The application of an external pressure, at least in principle, symmetrizes the MnO_6 octahedra, thus enhancing carriers mobility. In agreement with this oversimplified picture, a pressure-driven increase of the metal-insulator transition temperature T_{IM} has been observed in several manganites over a moderate pressure range (0-2 GPa). However in the high-pressure regime (P > 3-4 GPa) the $T_{IM}(P)$ curve bends down and seems to approach an asymptotic value. We have observed this behaviour in $La_{0.75}Ca_{0.25}MnO_3$ where $T_{IM}(P=0) = 220$ K). The high-pressure effect has been ascribed to the onset of a localizing mechanism which is competing with the natural pressure-induced charge delocalization. Using powder neutron diffraction we have determined the magnetic phase diagram and in particular the ferromagnetic transition temperature $T_C(P)$ line over a wide pressure range (0-9 Gpa). We compare it with the metal-insulator transition temperature $T_{IM}(P)$ determined with Raman scattering. We discuss whether the double exchange (DE) mechanism, which at P=0 is responsible for the close connection between the magnetic and the electronic transition, still holds in the high-pressure regime. At low temperature we observe the onset of antiferromagnetic order driven by the applied pressure. On the basis of both theoretical and experimental results we propose that an AF-SE coupling between the t_{2g} core spins could provide the high-pressure extra localizing channel.

The second system $LaMn_{0.7}Ga_{0.3}O_3$ belongs to a family of manganites $LaMn_{1-x}Ga_xO_3$ which show new and interesting magnetic and structural properties arising from a non Jahn-Teller (J-T) and no magnetic ion (Ga^{+3}) substituting for a J-T ion (Mn^{+3}). A surprising ferromagnetic insulator ground state is observed in the Ga-doping range $0.4 \leq x \leq 0.7$ which cannot be ascribed to a double-exchange (DE) mechanism because of the absence of hole doping. The undoped compound $LaMnO_3$ is considered as the prototype of a Jahn-Teller (J-T) system where a cooperative tetragonal deformation of the MnO_6 octahedra occurs. The $LaMnO_3$ structure can be viewed as a sequence of alternate short and long Mn-O bonds in the *ac* plane. Furthermore, the occurrence of orbital ordered states plays a fundamental role in stabilizing the anisotropic A antiferromagnetic state has also been established. All the structural studies on the Ga-doped compounds $LaMn_{1-x}Ga_xO_3$ show that the Ga substitution dramatically reduces the J-T distortion leading, for $x > 0.6$, to a crystallographic structure with all the MnO_6 octahedra in a symmetric configuration. Hydrostatic pressure has also been shown to symmetrize the MnO_6 octahedra whilst the magnetic structure at P = 0 Gpa is a canted antiferromagnetic structure of type A. We report the magnetic phase diagram as a function of an applied pressure for x = 0.3, which is still a distorted system, in a wide pressure range (0-6 Gpa) and compare it with our Raman scattering studies. At P = 0 GPa we observe an antiferromagnetic structure of type A (with the magnetic moments aligned along the *a*-axis) and a ferromagnetic contribution along the *b*-axis, in agreement with what previously found at ambient pressure. As pressure is applied, the system develops an antiferromagnetic component along the *b*-axis which is absent at ambient pressure. We discuss our findings in terms of 3*d* orbital fluctuations, which promote ferromagnetic order and e_g orbital ordering, which promote antiferromagnetic order.

Quantum rattling motion of hydrogen molecules in clathrate hydrate

Lorenzo Ulivi[(1)], Milva Celli[(1)], Alessandra Giannasi[(1)], Marco Zoppi[(1)], A. J. Ramirez-Cuesta[(2)]

[(1)] *Istituto dei Sistemi Complessi-CNR, Sez. Firenze, Sesto Fiorentino, Italy*
[(2)] *ISIS Facility, Rutherford Appleton Laboratory, Didcot, UK*

Clathrate hydrates are inclusion compounds, formed by a network of hydrogen-bonded water molecules that is stabilized by the presence of foreign (generally hydrophobic) molecules, hosted in cages of different form present in the structure. The stability of a binary clathrate hydrate with hydrogen as a guest molecule has been demonstrated recently [1,2]. These compounds can be synthesized at a pressure around 300 MPa. A different ternary clathrate hydrate compound, stable at much lower pressure, has been studied recently [3,4]. It consists of the classical sII structure (cubic, with 136 H_2O molecules per unit cell) stabilized by the presence of tetra-hydrofuran (THF). Besides the technological interest of these compounds as possible materials for hydrogen storage, they represent test materials to study the quantum dynamics of confined hydrogen molecules. In this talk the results of a recent inelastic neutron scattering measurements will be presented and discussed. The measurements have been performed on the TOSCA spectrometer at ISIS with molecular hydrogen into a heavy water clathrate, with completely deuterated THF. The high-resolution spectra recorded on TOSCA show unique features of the quantum dynamics of H_2. By a separation of ortho- and para-H_2 spectra, we are able to assign the spectral bands to rotational and center-of-mass translational transitions of either para- or ortho-H_2. The H2 molecule rotates almost freely, while performing a translational motion (rattling) in the cage, resulting a paradigmatic example of quantum dynamics in a non-harmonic potential well. Both the H_2 rotational transition and the fundamental of the rattling transition split into triplets, having different separation. The splitting is a consequence of a substantial anisotropy of the environment with respect to the orientation of the molecule in the cage, in the first case, or with respect to the center-of-mass position inside the cage, in the second case. The values of the transition frequencies and band intensities have been quantitatively related to the details of the interaction potential between H_2 and the water molecules, with a very good agreement. The study of such rotational dynamics of the single molecule and of possible clusters [4], will reveal details of the water-host intermolecular potential, that, in turn, will be useful to model the interaction and to calculate more practical conditions for the synthesis of hydrogenclathrate.

[1] Y.A. Dyadin *et al.*, *J. Struct. Chem.* **40**, 790 (1999).
[2] W. L. Mao *et al.*, *Science* **297**, 2247 (2002).
[3] L. J. Florusse *et al.*, *Science* **306**, 469 (2004).
[4] H. Lee *et al.*, *Nature* **434**, 743 (2005).

Structure and dynamics of PVME.
A neutron scattering and molecular dynamics simulation study.

S. Capponi[(1)], F. Alvarez[(1,2)], A. Arbe[(2)], J. Colmenero[(1,2,3)]

[(1)] *Departamento de Fisica de Materiales, UPV/EHU, Apdo 1072, 20080, San Sebastian*
[(2)] *Centro de Fisica de Materiales(CSIC-UPV/EHU), Apdo 1072, 20080 San Sebastian*
[(3)] *Donostia International Physics Center, Paseo Manuel de Lardizabal 4, 20018 Sebastian*

The joint use of neutron scattering (NS) measurements and fully atomistic molecular dynamics (MD) simulations is a powerful method to investigate the structural and dynamical properties of a glass-forming polymer such as poly(vinyl methyl ether) (PVME). Here we exploit this combination to study the short-range order details and the atomic motions well above the glass transition temperature. For this purpose, we have first verified the reliability of the simulated cell. We have simulated the static structure factor and compared it to that measured by neutron diffraction. Regarding the dynamical aspects, we have checked the results of MD simulations against quasielastic NS literature data on methyl group rotations [1] and on the hydrogen motions in the structural relaxation regime [2]. Once validated, the additional information provided by the MD simulations has been exploited to have a more precise insight into the short-range order and the atomic motions in this polymer. Finally, using this strategy, we are currently exploring also the influence of water on PVME dynamics. Preliminary results might be presented as well.

[1] A. Chahid, A. Alegría, J. Colmenero, *Macromolecules* **27**, 3282 (1994).
[2] J. Colmenero, A. Alegría, A. Arbe, B. Frick, *Phys. Rev. Lett.* **69**, 478 (1992).

Determinations of $S(Q,\omega)$ of liquid CD_4 revealing the molecular arrangement and the role of anisotropic interactions

G. Venturi[(1)], E. Guarini[(2)], F. Barocchi[(2)], M. Sampoli[(3)], U. Bafile[(4)]

[(1)] *CNR-INFM and CRS-Soft, c/o Dipartimento di Fisica Università di Firenze, Sesto Fiorentino, Italy*
[(2)] *Dipartimento di Fisica, Università di Firenze, Italy*
[(3)] *Dipartimento di Energetica, Università di Firenze, Italy*
[(4)] *Istituto dei Sistemi Complessi-CNR, Sez. Firenze, Sesto Fiorentino, Italy*

A detailed Molecular Dynamics (MD) study of the dynamic structure factor $S(Q,\omega)$ of liquid deuteromethane has been performed using four models for the site-site interactions of the methane dimer. Recent neutron inelastic scattering data and their comparison with the quoted MD results clearly show the efficiency of neutron dynamical measurements in the discrimination among possible methane potentials. By further investigating the salient differences in the anisotropic character of the interaction models used in our simulations, and by comparing their ability to reproduce the neutron inelastic spectra at low and intermediate Q values ($2 < Q < 15$ nm^{-1}), we could even individuate the preferential arrangement of the molecules in methane at liquid densities. Such unexpectedly rich and new outcomes of the combination of MD simulations with careful neutron dynamical measurements, is more than promising for the study and interpretation of the dynamic and static structure of more complex molecular liquids.

Studio comparativo della dinamica veloce di lisozima e DNA e ruolo dell'environment

Elena Cornicchi[(1)], Matteo Marconi[(1)], Giuseppe Onori[(1)], Alessandro Paciaroni[(1)]

[(1)] *Dipartimento di Fisica dell'Università di Perugia, CEMIN (Centro di Eccellenza per i Materiali Innovativi Nanostrutturati) and INFM CRS-SOFT, Via Pascoli 06123 Perugia, Italy.*

L'importanza fondamentale che le molecole biologiche hanno per ogni organismo vivente è strettamente legata alla loro funzionalità biologica. Proteine ed enzimi, così come il DNA, esercitano specifiche funzioni biologiche per le quali sono altamente specializzati e che richiedono una notevole flessibilità conformazionale da parte della macromolecola. Un contributo fondamentale per il raggiungimento di questa flessibilità è dato dalle fluttuazioni termiche, ovvero moti interni veloci con tempi caratteristici dell'ordine dei nano- e picosecondi ed ampiezze dell'ordine della frazione di Angstrom.
Utilizzando la tecnica dello scattering elastico di neutroni, abbiamo studiato questi moti veloci confrontando due biomolecole molto diverse fra loro, il lisozima, una piccola proteina globulare, e il DNA, intrappolate in matrici vetrose di glucosio-acqua. Le misure, realizzate sui due spettrometri backscattering IN13 e IN10, con diversa risoluzione in energia, sono state fatte in funzione del livello d'idratazione (g D_2O/g glucosio) e in funzione della temperatura. Affinità e differenze sono state rilevate tra le dinamiche delle due biomolecole.

Detailing the solvation layer composition of proteins in mixed solutions: a SANS study

R. Sinibaldi[(1)], M. G. Ortore[(1)], F. Spinozzi[(1)], F. Carsughi[(1)], P. Mariani[(1)]

[(1)] *Dipartimento di Scienze applicate ai Sistemi Complessi, Università Politecnica delle Marche, Ancona, Italy*

There is a big effort to investigate how non-aqueous solvents affect intermolecular forces, since certain co-solutes are stored in large concentrations in organisms living in conditions of stresses and play a key role in modulating protein stability. The understanding of the role played by hydration in activating protein intrinsic dynamics, as well as the link between preferential hydration, structural rearranging and biological functionality, requires a direct characterization of protein-solvent interface. We used SANS technique to investigate solvent composition near the protein surface, focusing our attention to a model protein, lysozyme, dissolved in water-glycerol [2] and in water-urea mixtures. Glycerol does not change secondary and tertiary structure of lysozyme and it has been found that lysozyme regains its catalytic activity even in nearly anhydrous glycerol with efficiency comparable with that in aqueous solutions. Urea is a well-known protein denaturant, despite its ubiquitous use, only little is known about the molecular mechanism underlying urea-induced protein unfolding. SANS experiments have been performed at Forschungerszentrum in Jülich (Germany) and at Hahn Meitner Institut in Berlin. As differences in the solvation shell were expected to be quite small, the experimental conditions to be investigated were selected on the basis of numerical simulations of SANS curves at different cosolvent composition and deuteration grades. Hence samples were prepared using convenient protein concentrations, cosolvent and deuterium amounts. A global fit method [2,3] has been used to estimate a thermodynamic model [4] that describes the exchange equilibrium of water and cosolvent between protein surface and bulk. The thermodynamic constants K obtained by the two set of experimental data clearly indicate that glycerol is preferentially excluded from lysozyme solvation shell, while urea is more concentrated in the solvation shell in respect to the bulk. The common fitted parameters, the K and the molecular volume of water in contact with protein surface, allow to estimate the preferential binding coefficient and the excess solvation number, as a function of co-solvent molar fraction. These results are in agreement with preferential interaction coefficient estimated with chemical/physical techniques. The most interesting result is the setting of a new method to investigate in detail proteins hydration features in mixed solvents via SANS experiments, resulting to be able to confirm that stabilizing and denaturing effects due to the presence of a cosolvent are strictly correlated to their affinity with the protein surface.

[1] T. Knubovets *et al.*, Proc. Natl. Acad. Sci. **96**, 1262-1267 (1999).
[2] R. Sinibaldi, M. G. Ortore, F. Spinozzi, F. Carsughi, H. Frielinghaus, S. Cinelli, G. Onori, and P. Mariani, *J. Chem Phys.* **126**, 235101 (2007)
[3] M.G. Ortore *et al.*, *Chem. Phys. Lett.* **418**, 342-346 (2006)
[4] J. A. Schellmann, *Biophys. J.* **85**, 108-125 (2003)

Studying the low-frequency vibrational features of water at the interface with a deuterated protein.

A. Paciaroni[(1,2,3)], A. Orecchini[(1,2)], E. Cornicchi[(1,2,3)], M. Marconi[(1,2,3)], C. Petrillo[(1,2)], F. Sacchetti[(1,2)], M. Haertlein[(4)], M. Tarek[(5)]

[(1)] *Dipartimento di Fisica, Università degli Studi di Perugia*
[(2)] *Soft INFM-CNR*
[(3)] *CEMIN Perugia*
[(4)] *Deuteration Laboratory, ILL, Grenoble*
[(5)] *CNRS, Nancy*

We report a neutron scattering investigation focussed on the vibrational behaviour of the Maltose Binding Protein (MBP) and its hydration water in the picosecond timescale, i.e. the timescale of low-frequency collective motions. Due to the very high cross section of hydrogen atoms, neutron scattering is a very suitable technique to investigate the dynamical properties of biomolecules in the picosecond timescale. At low hydration degree the contribution from the deuterated solvent can be reasonably neglected, thus allowing to single out directly the protein spectrum. On the contrary, the signal from the sole solvent can be plausibly measured in presence of a perdeuterated protein sample. To properly separate the protein and solvent low-frequency contributions, we therefore measured protonated MBP+D_2O, deuterated MBP+H_2O and protonated MBP+H_2O, by means of the time-of-flight spectrometer IN5.
The signature of a strong coupling between the protein and hydration water vibrational dynamics is found around 3 meV. The density of states of protein hydration water can be decomposed in terms of the density of states of high- and low-density amorphous ice (HDA and LDA respectively), with the large predominance of HDA ice.

A new physical approach to understanding demyelization: investigation of the structure and dynamics of model myelin sheaths

De possibilitate vitam biologicam studere rigore et patientia

Alessio De Francesco[(1)]

[(1)] *CNR-INFM and CRS-Soft, c/o Institut Laue-Langevin, Grenoble, France*

The myelin sheath is a membrane of the peripheral nervous system which acts as an electrical insulator around the nerve axons. This membrane, whose task is to increase the speed of the neural signals, is composed of a complex structure of lipids and proteins organised in a multilayer structure [1]. Its degradation (demyelization) is observed in diseases like Multiple Sclerosis, where the myelin structures breaks down without evident damage to the underlying axon [1].
It is known that this illness is caused by an autoimmune response against one or more myelin antigens triggered by a combination of genetic predisposition and environmental factors. The latter is thought be caused by viral infections in early stages of the individual's life. The autoimmune response could be related to similarity in the primary sequence between some viral proteins and proteins presents in the myelin (myelin basic protein [2], proteolipid protein [3]) or between lipidic components [4]. However, neither a unique and specific MS virus, nor definitive antigens have been identified, and the combination of more of these candidates might instead have a "catalytic role" on the onset of the illness [1].
It is therefore essential to acquire a detailed knowledge of the physical chemical properties of myelin, and of its structure and organization in order to reveal how and why specific antigens become selected from the antibodies. Neutron and X-ray reflectometry are powerful means to elucidate structural aspect of the multilayers adsorbed on planar substrates due to their sensitivity to surface properties.
Other aspects to be tackled are collective dynamical issues related to the demyelinization process. The structural changes occurring in this case resemble the biophysical changes occurring in membrane fusion and adhesion, where (collective) changes in curvature play a relevant role [5]. Collective dynamics have become visible recently by Inelastic Neutron Scattering experiments [6]. These experiments performed by varying the content and the type of the myelin proteins could shed light in what determine the stability and the instability of these systems with obvious benefit in the understanding what can favour and hinder demyelinization.
A possible problem that could be encountered in this study is how close a myelin system on a model surface could represent the real myelin system, since its "in vivo" structure and functionality are highly dependent on interactions with the underlying axons. An adequate interfacial cushion that could mimic "in vivo" conditions should therefore be developed in collaboration with biology groups and expertise in the field of neurology. Preliminary contacts made through the McGill Neuroengineering Center (constituted of researchers in Chemistry, Physics and the Neurological Institute) reveal that efforts to create highly biomimetic "in vitro" cell growth condition are well underway.

[1] K. A. Williams, C. M. Deber, *Critical Reviews in Clinical Laboratory Sciences* **30** (1), 29-64 (1993).
[2] Oldstone, *Cell* **50**, 819 (1987).
[3] S-Y. Shaw, R. A. Laursen, M.B. Lees, *FEBS Lett.* **207**, 266 (1986).
[4] N. Kasai, A. R. Pachner, R. K. Yu, *J. Neurol Sci.* **75**, 33 (1986).
[5] B. Ohler, K. Graf, R. Bragg, T. Lemons, R.Coe, C. genian, J. Israelachvili, C. Husted, *Biochimica and biophysica Acta* **1688**, 10 (2004).
[6] M. C. Rheinstädter, C. Ollinger, G. Fragneto, F. Demmel, and T. Salditt, *Phys. Rev. Lett.* **93**, 108107 (2004).

Microscopic structure of single walled carbon nanotubes and allotropic impurities

Milva Celli[(1)], Alessandra Giannasi[(1)], **Marco Zoppi**[(1)]

[(1)] *Istituto dei Sistemi Complessi-CNR, Sez. Firenze, Sesto Fiorentino, Italy*

Pulsed neutron diffraction has been used to characterize the microscopic structure and purity of single walled carbon nanotubes samples produced by arc discharge. We used the SANDALS time of flight diffractometer, whose performance in measuring the microscopic structural properties of light-mass materials is well known and recognized. The extended Q-range of the instrument allows for a direct inversion of the data to determine the radial distribution function of the carbon atoms. This is compared with the corresponding function produced by computer simulation. In addition, the absolute calibration of the neutron diffraction data evidences anomalies in the diffraction spectra of the carbon nanotubes, especially at the level of the total scattering section, that could not be observed in previous neutron scattering experiments. These are attributed to the presence of a substantial amount of spurious carbonaceous material that was not quantitatively detected with more conventional diagnostic techniques.

Poster

Large wave vectors sound excitations in the collective dynamics of fluids

U. Bafile[1], F. Barocchi[2], E. Guarini[2], M. Sampoli[3], G. Venturi[4]

[1] *CNR Istituto dei Sistemi Complessi, sezione di Firenze, Firenze, Italy*
[2] *Dipartimento di Fisica, Università di Firenze, Italy*
[3] *Dipartimento di Energetica, Università di Firenze, Italy*
[4] *CNR-INFM and CRS Soft, c/o Dipartimento di Fisica, Firenze, Italy*

A two-decade development of dedicated high-performance instrumentation at major neutron and synchrotron radiation sources has stimulated numerous spectroscopic studies of the collective dynamics of fluids, rising the neutron and x-ray versions of Brillouin scattering to well-established and fruitful experimental methods in this field. However, in contrast with the large amount of dynamical studies performed at wave vectors Q below the position Q_p of the main peak in the static structure factor $S(Q)$, very little is known about the behaviour of acoustic excitations at quite larger Q values. We present molecular-dynamics simulation results for the translational part of the dynamic structure factor of the molecular liquid CD_4 up to rather high wave vectors ($Q \sim 4Q_p$), analyzed by means of the viscoelastic model line shape. Our investigation shows that underdamped sound modes persist up to such high Q values, in agreement with a non-vanishing *distinct* part in $S(Q)$, with the exception of a restricted interval around Q_p where the collective oscillations undergo a transitory overdamping.

Water diffusivity in PVA-based transdermal patches

C. Chiapponi[1], M.T. Di Bari[1], A. Deriu[1], F. Sonvico[2], P. Santi[2], S. Nicoli[2], C. Padula[2], J. Ollivier[3]

[1] *Università di Parma, Dipartimento di Fisica and CNISM, Parma, Italy*
[2] *Università di Parma, Dipartimento Farmaceutico, Parma, Italy*
[3] *ILL, Grenoble, France*

Transdermal patches are innovative drug delivery systems intended for skin application. We present here the results of a QENS experiment on a water-based and vapor permeable bioadhesive film intended for dermal/transdermal delivery. The film is obtained by mixing water solutions of a film-forming polymer (polyvinyl alcohol), a water-soluble adhesive, a plasticizer (glycerin or sorbitol) and a model drug. The resulting solution is laminated on siliconized paper and oven dried at 80 °C. The obtained film is not adhesive in the dry state but only when applied on wet skin. Film-water interaction is a key factor for the behavior of the film itself. This is supported by the following observations: i) the film becomes adhesive only when in contact with water; ii) the efficiency of drug release from the film depends on the amount of water applied; iii) the film is highly water permeable (1500 g m^{-2} in 24 hrs) and water soluble.
Using the TOF spectrometer IN5 at the ILL we have measured quasielastic scattering spectra of the film at room temperature and at several hydration levels from the almost dry state up to about 50% water content (by weight) that corresponds to the conditions of medical application. The effect of the presence of a drug has also been investigated loading the film with a model drug (lidocaine, ~ 8% by weight).
Up to about 14% hydration the quasielastic spectra are similar in shape to that of the dry sample indicating that most hydration water is bound to the film. Further water addition gives rise to a broad quasielastic component due to water molecules weakly bound to the film, and with properties similar to those of bulk water. Addition of lidocaine does not change significantly the diffusivity properties of hydration molecules.

The Italian Neutron Experimental Station (INES) at ISIS: status and development

Francesco Grazzi[(1)], Laura Bartoli[(1)], **Milva Celli**[(1)], Silvia Imberti[(2)], Marco Zoppi[(1)]

[(1)]ISC-*CNR, Sesto Fiorentino (FI), Italy*
[(2)]*ISIS-RAL, Chilton, Didcot (OXON), Great Britain*

The INES project concerns the realization of a multipurpose experimental station, built by CNR at the ISIS pulsed neutron source (Rutherford Appleton Laboratory, UK). This instrument is mainly intended to operate as test and training facility for the Italian neutronscattering community. The experimental station is equipped with a multipurpose time-of-flight neutron diffractometer. This is located downstream a water moderator of the neutron source, with an excellent time-resolution. In the present configuration the INES
diffractometer contains a highly-efficient large detector area covering a range of about 170° on the horizontal plane. Moreover it offers a large sample volume (about 0.25 m^3), allowing the study of almost any kind of object, including bulky archaeological artifacts. The possibility to separately analyze each single detector makes texture analysis also possible. The opportunity to operate experiments in particular thermodynamic conditions (i.e. high pressure, high and low temperatures) is also under investigation.

Neutron scattering determination of the dynamic structure factor of liquid CO_2

R. Favillini[(1)], U. Bafile[(2)], F. Barocchi[(1)], F. Formisano[(3)], E. Guarini[(1)], A. Orecchini[(4)], M. Sampoli[(5)], G. Venturi[(6)]

[(1)]*Dipartimento di Fisica, Università di Firenze, Italy*
[(2)]*CNR Istituto dei Sistemi Complessi, sezione di Firenze, Italy*
[(3)]*CNR-INFM and CRS Soft, c/o Institut Laue Langevin, Grenoble, France*
[(4)]*Dipartimento di Fisica, Università di Perugia, Italy*
[(5)]*Dipartimento di Energetica, Università di Firenze, Italy*
[(6)]*CNR-INFM and CRS Soft, c/o Dipartimento di Fisica, Firenze, Italy*

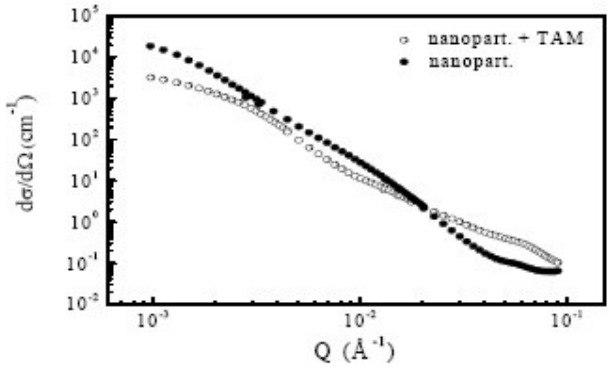
We report on a recent neutron inelastic scattering measurement of the dynamic structure factor of liquid carbon dioxide in the range $1.5 < Q < 17$ nm^{-1}. After a detailed data treatment, including the usual corrections for background, attenuation and multiple scattering, experimental spectra have been compared with molecular dynamics simulations using up to four different site-site model potentials. Within the instrumental resolution, all used models reasonably describe the observed dynamics. However, there are indications that all trial interaction models slightly, though systematically, overestimate the damping of the collective modes, as soon as the hydrodynamic regime is abandoned ($Q > 3$ nm^{-1}). The experience recently gained about the connection of collective properties with the interaction features in another molecular liquid, namely deuteromethane, may suggest that the model potentials we employed for CO_2 suffer from an excessively hard short-range behaviour.

Neutron investigation of the structure and organisation of phospholipid/saccharide nanoparticles

Y. Gerelli[(1)], M.T. Di Bari[(1)], A. Deriu[(1)], F. Sonvico[(2)], C. Como[(2)], P. Colombo[(2)], R. May[(3)]

[(1)] *Università di Parma, Dipartimento di Fisica and CNISM, Parma, Italy*
[(2)] *Università di Parma, Dipartimento Farmaceutico, Parma, Italy*
[(3)] *Institut Laue-Langevin, Grenoble, France*

In recent years nano- and micro-particles composed of polymeric or lipid material have been proposed as drug carriers to improve the biological availability and hence the efficacy of the encapsulated drug. For the production of these delivery systems a number of different materials have been proposed, such as polysaccharides, synthetic polymers, lipids etc. Among them phospholipids and polysaccharides have received a considerable attention due to their biocompatibility, biodegradability, low cost, and safety.
The understanding of the structure and of the interactions involved in nanoparticle formation has major relevance for the tailoring of the properties of the carrier and of the release of the drug in order to obtain specific therapeutic effects. We report here the results of a structural investigation, performed using D11 at the ILL, on nanoparticles (typical average size 100 nm) prepared by self-assembling of phospholipids (soybean lecithin) in aqueous medium containing a fixed amount of chitosan, a positively charged polysaccharide. The SANS data indicate the presence of an inner region of about 60 nm mostly occupied by the solvent surrounded by a lipid shell ~ 5 nm thick. Chitosan provides an outer coating that contributes to the particle stability. In the experiment we investigated also the effect of the addition of tamoxifen (TAM), a positively charged drug used in breast-cancer treatments. The presence of tamoxifen induces a important structuring of the lipid component of the nanoparticles that is revealed by the appearance of a broad peak at about ~ 0.06 $Å^{-1}$ that can be ascribed to the formation of a relatively regular multilayer structure in the lipid component of the nanoparticles.



Small Angle Neutron Scattering characterisation of Al_2O_3/Ni-P nanocomposites

F. Rustichelli[(1)], F. Fiori[(1)], C. Renghini[(1)], **E. Girardin**[(2)], G. Albertini[(2)], K. Konopka[(3)]

[(1)] *Università Politecnica delle Marche, Dipartimento SASC (Sezione di Scienze Fisiche), Via Brecce Bianche, 60131 Ancona, Italy*

[(2)] *Università Politecnica delle Marche, Dipartimento FIMET, Ancona, Italy*

[(3)] *Faculty of Materials Science & Engineering, Warsaw University of Technolgy, Woloska 141, 02-507 Warsaw, Poland*

Small Angle Neutron Scattering (SANS) investigation of the distribution of the metallic particles in hot pressed Al_2O_3/Ni-P nanocomposites has been carried out at the PAXE instrument of the Laboratoire Léon Brillouin - C.E.A., Saclay, France. The goal of this experiment was to get information about the morphology of the metallic particles. In particular, their size and fractal behaviour were determined, as functions of the sintering temperature.

-alumina powder with an average grain size of 2.5 μm and a purity of 99.5% was used in the experiment. The powder was plated with an Ni-P alloy in an electroless nickel or boron bath. After drying, the plated powder was sintered at various temperatures (Room temperature, 600°C, 800°C, 1000°C) via a hot-pressing method under a pressure of 7 GPa. The samples were obtained in the form of cylinders, 5 mm in diameter and 3 mm in height. According to previous characterizations, the coated powder consisted of ~28 wt.% of Ni-P, which contained ~2wt.% of P. The layer was made up of nano-aggregates of particles having a diameter close to 10 nm at room temperature growing with the sintering temperature.

The investigated scattering vector (Q) range was 0.006 $Å^{-1} < Q < 0.1$ $Å^{-1}$. The low- Q behaviour allows the determination of the Guinier (gyration) radius R_G of the particles; in particular it can be shown that the curve $(d\Sigma/d\Omega)\,Q^2$ versus Q, where $(d\Sigma/d\Omega)$ is the SANS cross section, has a maximum at $Q=3^{1/2}/R_G$, so that R_G can be obtained by fitting the theoretical curve to the experimental data. In the case of spherical particles $R_G^2=3/5\,r^2$ and so the radius of the sphere is $r=(5/3)^{1/2}\,R_G$, giving r = 12 nm at RT, in agreement with SEM observations. For higher sintering temperatures the particles tend to coarse, so that they are not spherical anymore and the evolution of their Guinier radius is determined by both their size increase and geometry change.

At larger Q, the scattered intensity obeys a power law describing the surface geometry. When flat, the power has the value of -4 (Porod's law); when fractal, it deviates, taking a value between -4 and -3. An object is said to be a fractal when it shows a scale invariance over a certain length range. In the case of a surface: $S \propto R^{Ds}$ where S is the area of the surface, R the radius of the object and D_s the surface dimension. The surface fractal dimension D_s is linked to the minimum number N of balls of radius a needed to cover a surface completely. For a fractal surface: $N=N_0\,a^{-Ds}$, where $2<D_s<3$.

In the case of SANS from fractal surfaces $(d\Sigma/d\Omega) \propto Q^{Ds-6}$, so that the surface fractal dimension D_s is obtained by the curve slope in a logarithmic scale.

Results show that the surface fractal dimension decreases with the increasing sintering temperature. This is in accordance with the microscopic observations: at room temperature the metallic particles are spherical and, as stated above, as the sintering temperature increases the particles are melted, thus approaching a more "flat" surface shape.

Etruscan weapons investigated through neutron radiography and diffraction

R. Magli[1], S. Bianchi[2], G. Andrè[3], M. Benvenuti[2], P. Costagliola[2]

[1] *Dipartimento di Chimica, Biochimica e Biotecnologie per la Medicina, Università di Milano, Italy*
[2] *Dipartimento Scienze della Terra, Università di Firenze, Italy*
[3] *Laboratoire Léon Brillouin, (CEA-CNRS) CEA Saclay, France*

Populonia (southern Tuscany, Italy) represented a very important metal production centre during Etruscan (7th-3rd century BC) and Roman (2nd century BC – 2nd century AD) times. Notwithstanding production of iron, copper, bronze and other metal artefacts is archaeologically well established, still many aspects await better definition in terms of metallurgical technologies, provenances of raw metals, trade exchanges with other towns from Etruria and elsewhere, partly because of the scarcity of well preserved items from local workshops. The objects analysed in this study came to light just underneath the Populonia acropolis, as the sea eroded away part of a large deposit of metallurgical debris extending along the shoreline. The deposit (approx. 70x78x28 cm) is composed of several iron and bronze weapons, most of which strongly welded by corrosion products. Bronze artefacts are relatively well preserved whereas iron objects are covered by thick coatings of alteration products. The present project aims to fully characterize the various items from a morphological, compositional and technological point of view. Due to the high archaeological value of the finding and to its complex nature and morphology, an exhaustive investigation can be performed only through the use of different and complementary non-destructive analytical means.
Neutronography has been beneficial for getting information about the general shape and also the content of the single artefacts constituting the deposit. In order to perform a comprehensive composition study also a neutron diffraction analysis has been performed using the G4.1 (LLB) diffractometer. The data have been processed by applying standard Rietveld refinements in order to get a qualitative and quantitative mineralogical composition of the investigated items. We report and discuss here the results of the analysis performed up to now.
Further analysis, including an investigation of the residual stresses fields possibly still present as well as a texture evaluation of the samples are shortly foreseen at ILL. We expect that the results, together with neutronography and diffraction data, can provide useful hints to identify the metalworking techniques and, by comparison with data obtained for coeval and/or similar weapons, to define possible evolutionary trends in Etruscan metallurgy. This could have obvious relevant implications from a strictly archaeological point of view; hopefully, it could also represent a starting point for application of such techniques to the study of so complex archaeo-metallurgical objects.

Combined SANS/SAXS study of the BSA solvation layer in urea aqueous solutions

M. G. Ortore[1], R. Sinibaldi[1], F. Spinozzi[1], P. Mariani[1]

[1] *Dipartimento di Scienze applicate ai Sistemi Complessi, Università Politecnica delle Marche, Ancona, Italy*

We present a set of SANS and SAXS experiments concerning Bovine Serum Albumine (BSA) in urea-water mixtures, before the unfolded state. A new method able to quantitatively determine the composition of the solvation shell of proteins in a mixture [1] has been successfully applied to the case of BSA. Both SANS and SAXS experiments were performed with different protein concentration values and urea molar fractions in solution. Each set of SAS experiment was analysed using a global fit strategy, by means of a thermodynamic model that describes the exchange equilibrium between molecules in the bulk and in protein solvation shell [2]. This study confirms the efficiency of the new methodology applied to both SANS and SAXS experiments, it proves that urea prefentially binds to protein surface in every experimental conditions and describes in detail how protein-protein interactions are modified by the presence of urea in solution.

[1] R. Sinibaldi, M. G. Ortore, F. Spinozzi, F. Carsughi, H. Frienlinghaus, S. Cinelli, G. Onori, and P. Mariani, *J. Chem Phys.* **126**, 235101 (2007).
[2] J. A. Schellman, *Quat. Rev. Biophys.* **38**, 351 (2005).

Dynamics in an ultra fragile glass former: Decalin

M. Plazanet[1,2], S. Eibl[2], H. Schober[2]

[1] *LENS, Firenze, Italy*
[2] *Institut Laue-Langevin, BP 156, Grenoble, France*

The microscopic dynamics of the glass former cis-Decalin has been investigated by inelastic and quasi-elastic incoherent neutron scattering giving the single particle self-correlation function. The non-ergodicity parameter, low-frequency vibrational dynamics and fast relaxation dynamics are reported here. Both in the glass and in the crystal the vibrations show strong anharmonic behavior. In the glass phase, the short time microscopic dynamics evolve rapidly with temperature, however do not exhibit any significant change around T_g. The cusp behavior predicted by the Mode Coupling Theory is particularly well observed, which enables the determination of the critical temperature T_c = 146.5 K. This is only 1.07 times higher than T_g. The mean square displacements are comparable to those measured in other fragile glass formers, although the temperature is much lower in the present case. The beta relaxation is clearly visible and discussed in the framework of the Mode Coupling Theory and the fragility concept. The results are put into context with respect to the archetypical fragile glass OTP.

Interaction between amyloid aggregates and phospholipid membranes: a neutron diffraction study

Silvia Dante[1], Annalisa Relini[2], Silvia Torrassa[2], Thomas Hauss[1], Monica Bucciantini[3], Massimo Stefani[3], Alessandra Gliozzi[2], **Ranieri Rolandi**[2]

[1] *Hahn-Meitner-Institut GmbH, Abteilung SF2/Biophysik, Berlin, Germany*
[2] *University of Genoa, Department of Physics, Genoa, Italy*
[3] *University of Florence, Department of Biochemical Sciences, Florence, Italy*

Amyloid aggregation is involved in several fatal diseases, such as Alzheimer's disease, Parkinson's disease and systemic amyloidoses. Increasing experimental evidences indicate that protein oligomers, rather than mature fibrils are the major responsible of cytotoxic effects through the interaction with cell membranes.
HypF-N (MW 10452 Da) is the N-terminal domain of a bacterial hydrogenase maturation factor. This protein undergoes amyloid aggregation in the presence of trifluoroethanol (TFE) and its pre fibrillar aggregates are toxic to cultured cells. Therefore, it represents a useful model to study fibrillogenesis and the interaction of prefibrillar and fibrillar aggregates with cell membranes. In this work we use neutron diffraction to study the interaction of HypF and its amyloid aggregates with phospholipid membrane models. Neutron diffraction measurements have been carried out at BENSC with the V1 diffractometer on POPC/POPS (92:8 mol/mol) supported membranes containing native, oligomeric and fibrillar HypF. POPC/POPS liposomes were incubated either with HypF in the native state, oligomeric HypF obtained after 22 h aggregation or HypF mature fibrils obtained after 7 days. After incubation, liposomes were deposited onto quartz slides and dried using a laminar flux hood. Samples were prepared using both non deuterated HypF and HypF carrying 35 deuterated glycines.
The preliminary analysis of the results shows that the structure of the lipid bilayer is strongly affected by the interaction with the protein. The pure lipid sample is constituted by well ordered lamellar structures with low mosaicity as shown by the sharp reflections detectable up to the fifth order. The presence of the protein suppresses reflections higher than the third order and increases sample mosaicity. Mosaicity was strongly increased in the presence of native HypF; this effect was smaller in the presence of HypF oligomers and further reduced in the presence of HypF fibrils. Interestingly, in the presence of amyloid fibrils, reflection shapes indicate a broadening of the spacing Gaussian distribution. This effect could be due to the presence of a new spacing very close to, but different from that of the phospholipid bilayer. This behavior, which is absent in the presence of native HypF, is observed at a lesser extent with oligomers.