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30 Giugno – 1 Luglio 2008
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Comitato Scientifico:
M. Celli, A. Deriu, E. Guarini, S. Magazù, R. Magli,
P. Mariani e A. Orecchini

ABSTRACT BOOK

PROGRAMMA

Lunedì 30 Giugno 2008

8:45 – 9:00	Introduzione e benvenuto
9:00 – 10:00	R. Caciuffo *“Superconductivity without phonons in PuCoGa$_5$?”*
10:00 – 11:00	P. Timmins *“Structural biology and neutrons – the shape of things to come”*
11:00 – 11:30	Coffee Break
11:30 – 12:00	Premio per la miglior Tesi di Dottorato di Ricerca su Tematiche di Spettroscopia Neutronica: T. Guidi *“Spin excitations and magnetic properties of molecular nanomagnets”*
12:00 – 12:30	C. Chiapponi *“Influence of gangliosides on membrane dynamics”*
12:30 – 13:00	Y. Gerelli *“Lipid/polysaccharide nanovectors for drug delivery”*
13:00 – 14:30	Pranzo
14:30 – 16:30	Sessione Poster (con *Clip-Session*)
16:30 – 17:00	Coffee Break
17:00 – 19:30	Assemblea SISN
20:30	Cena sociale

Martedì 1 Luglio 2008

8:30 – 9:30	D. Bowron *“From SANDALS to NIMROD: new opportunities for structural studies of liquids and disordered materials over atomic to mesoscopic length scales”*
9:30 – 10:00	C. Ziparo *“QENS measurements on AOT- water- decane microemulsion.”*
10:00 – 10:30	L..Orsingher *“Vibrational density of states in densified GeO$_2$ glasses”*
10:30 - 11:00	Coffee Break
11:00 – 11:30	M.G. Ortore*“Lysozyme in water-ethanol mixtures: preferential hydration and consequent unexpected phenomena”*
11:30 – 12:30	Incontro con i responsabili Italiani di strumenti “CRG“: *BRISP (A. De Francesco), IN13 (F. Natali), INES (L. Bartoli)*
12:30 – 12:45	Premiazione Poster e Relazioni di giovani ricercatori.
12:45	Saluti e chiusura del congresso

RELAZIONI SU INVITO

Experimental investigation of structure in liquids and disordered materials, the path from atomic to mesoscopic length scales

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Understanding the structure of liquids and disordered materials is important if we wish to improve our ability to tailor the physical, chemical or materials properties of many systems of modern technological interest. Over the past few decades neutron scattering techniques have played an important role in advancing this knowledge and increasingly, when these methods are combined with modern computational capabilities, they are providing unprecedented insight into the details of atomic and molecular interactions. Following the growth in the structural complexity of today's scientific challenges it is increasingly becoming necessary to relate physical and chemical processes across a wide range of length scales. This requirement has motivated the development of new instrumentation, for example the Near and InterMediate Range Order Diffractometer (NIMROD) at the ISIS second target station. This talk will illustrate, using a relatively simple tertiary butanol – water solution [1], how techniques have evolved to date, and where they may develop in the future.

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Superconductivity without phonons in $PuCoGa_5$?

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The discovery of *d*-wave superconductivity in $PuCoGa_5$ at the surprisingly high critical temperature of T_C = 18 K [1] raised much interest, and triggered extensive research on the many complex and diverse phenomena which have been observed in the series of isostructural RMX_5 intermetallic compounds (R = cerium or light actinide element; M = transition metal element; X = element of the boron group) [2, 3]. Current research on this family is enhanced by the possibility to explore links between unconventional superconductivity, magnetism, and non-Fermi liquid behavior in proximity of a quantum critical point [4]. No long-range magnetic order is observed in $PuCoGa_5$, but theoretical work [5-8] as well as recent NMR experiments [9] suggest the presence of spin polarization and hence strong magnetic correlations. On the other hand, convincing evidence that spin fluctuations really act as pairing boson for superconductivity is still lacking [10], mostly due to the fact that no direct measurement of the magnetic fluctuation spectra has yet been reported. Inelastic neutron scattering is the technique of choice to address this problem, but the large neutron absorption cross-section of ^{239}Pu, and the lack of large single crystals of $^{242}PuCoGa_5$ do not allow such experiments at the moment. Nevertheless, useful hints on the spin fluctuations of $PuCoGa_5$ can be inferred from the magnetic excitations in the isostructural antiferromagnetic compound $NpCoGa_5$; this compound shows antiferromagnetic order below T_N = 47 K, with an ordered magnetic structure on the Np sublattice defined by the propagation vector (0 0 1/2). This is exactly the reciprocal space position where theory predicts the dominant weight for the magnetic fluctuations in $PuCoGa_5$ [7].

Here we present the results of polarised neutron diffraction experiments [11] performed on the hot neutron diffractometer D3 at the ILL using single crystals of m = 160 mg and m = 125 mg of the superconductor $^{242}PuCoGa_5$ and its isostructural homologue $NpCoGa_5$. Inelastic neutron scattering experiments performed on $NpCoGa_5$ [12] are also discussed. Our results show that the *normal* state of $PuCoGa_5$ is substantially different from that anticipated from a conventional Pu^{3+} ion, which would exhibit Curie-Weiss-like behaviour in the normal state. The absence of a sizeable paramagnetic moment on the plutonium sites is a new fact that must be considered when assuming Cooper pairing mediated by spin-fluctuations. In $NpCoGa_5$, our experiment gives evidence for the existence of two energy scales for the magnetic excitations in the ordered phase; one is related to a non-dispersive excitation between two crystal field levels (with a bare gap modified by mean-field exchange), and another corresponds to dispersive spin fluctuations emanating from the magnetic zone centre and associated to non-local excitations persisting in the paramagnetic phase. This fact would support the possibility that magnetic fluctuations centered around (0 0 1/2) are present also in $PuCoGa_5$, where they have been proposed as a possible mediating boson responsible for the appearance of superconductivity [14]. However, alternative scenario cannot be excluded and an interpretation of the available data in the framework of the Eliashberg theory of superconductivity will be discussed.

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Structural Biology and Neutrons – the Shape of Things to Come

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Biology is currently undergoing a revolution both in terms of new discoveries as well as the way in which we approach its study. We are moving into the area whereby a much more integrative rather than reductionist approach is taken to understanding the functioning of living systems. Moreover, the use of multiple techniques is more and more important. Where can neutrons play a role in this research? Neutrons are extremely versatile – they can probe both structure and dynamics, they can probe the bulk and surfaces, solutions and solids. All these properties are of importance for biology.

In this presentation I shall deliberately talk only of structure, being the basis upon which all other properties depend. The improvements in technology at current sources, stimulated by developments taking place at new and future sources is giving a new impulse to biological research with neutrons.

It is now possible to study crystals of biological macromolecules in order to locate hydrogen atoms so vital to catalytic processes. With the study of larger and larger complexes it is rapidly being realized that a whole battery of techniques is required to determine structures. Hence for example high resolution information from X-ray crystallographic studies of component molecules can be used in conjunction with neutron small angle scattering to elucidate the structure of large functional complexes which by their nature cannot be crystallised. The study of membranes is of vital importance both to the understanding of biological function and in human health where they represent the majority of drug targets. Neutron reflectometry is a technique perfectly adapted to the study of such systems and with instrumental and flux improvements of the coming years is set to make a major contribution beyond the field of model membranes into the domain of real biological membranes.

PREMIO SISN PER LA MIGLIOR TESI DI DOTTORATO DI RICERCA SU TEMATICHE DI SPETTROSCOPIA NEUTRONICA

(cicli XVII-XX)

Spin Excitations and Magnetic Properties of Molecular Nanomagnets

Presentata da: Tatiana Guidi

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In this thesis work the spin dynamics of several molecular cluster compounds have been studied in detail.
INS spectroscopic techniques have been intensively used to directly access the energies and eigenfunctions of the different spin states of the clusters, thus contributing information very useful to build a comprehensive picture of their magnetic anisotropy and quantum-mechanical behavior. INS experiments on Fe4-OMe cluster have given a clear-cut answer on the lowering of symmetry that was suggested by previous results. On the contrary, the same kind of experiments on Fe4-thme variety have shown that selective substitution of ligands in the molecule can raise the symmetry and the anisotropy barrier. This result opens new perspectives on the possibility to use subtle chemical changes to optimize the properties of new materials. Moreover, the accurate determination of the microscopic Hamiltonian has clarified the origin of the observed tunneling behavior that was until now unexplained.
The interplay between theoretical and experimental results on various cyclic polynuclear wheels (Cr8, Cr7M, Fe10) have given exciting results both for the modelling of linear AF chains and for the potential technological applications. We have shown that the lowest magnetic excitations in these AF wheels are not the classical spin waves but quantized rotations of the Néel vector. The dynamics of this newly observed phenomenon have been investigated in detail. Moreover, the experimental determination of the eigenvalues and eigenfunctions of substituted Cr7M wheels revealed the presence of favorable conditions for observing QT of the Néel vector and for the implementation of the qubit. Finally, we have measured the spin excitations of a 3*x*3 grid complex, Mn[3*x*3], and the resulting spin Hamiltonian has been used to explain unexpected oscillations in the mag-netic torque signal. This effect has been ascribed to a new quantum tunneling mechanism, associated with the mixing of different S states. These new phenomena are of fundamental importance, and may underpin future technologies such as Quantum Information Processing.
Chemists are ever continuing to push for new and more advanced molecular configurations of the clusters, which presents a constant challenge to Physicists to provide the theoretical description of these systems.

COMUNICAZIONI ORALI

Influence of gangliosides on membrane dynamics

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Glycolipids are an important part in the class of amphiphilic molecules and are abundant in animal cell plasma membranes. They are thought to play an important role in processes such as cell recognition, protein binding and signal transduction. Their feature is the presence of sugar groups in the hydrophilic head.

The most complex variety of glycolipids is represented by gangliosides, in which there are one or more sialic acid residues in the sugar head: the consequence is a significant steric hindrance and a net electrostactic charge under physiological conditions; due to this charge gangliosides act an important role in ion distribution across the membrane.

In recent years a lot of interest has developed around gangliosides-rich domains in monolayers and bilayers. The system here presented is a phospholipidic oriented membrane made by 1,2-Dimyristolyl-*sn*-Glycero-3-Phosphocholine, DMPC, in which the "prototype" gangliloside monosialotetrahexosylganglioside, GM1, has been added: GM1 has particularly important physiological properties in neuronal plasticity and repair mechanisms and it is also related with the release of neurotrophins in the brain.

Several neutron scattering experiments have been done on such a system: the interest is to understand if the presence of the ganglioside induces any effects on the dynamics of the oriented membrane. Results of two particular experiments will be presented. Firstly an elastic experiment on the high-resolution backscattering spectrometer IN13 at ILL in Grenoble: these measurements show that over a certain level of sample hydration no anisotropy and GM1 dependence are observed in the low T region, i.e. up to 320K; for temperature higher than 320K an abrupt increase of the mean square displacement, as calculated for the Q dependence of the elastic intensity at low Q, appears and with it a strong anisotropic effect divides the behaviour of the in plane motions from the out of plane ones.

To complete these results, a further analysis has been performed by quasi-elastic neutron scattering experiment, done on the time-of-flight spectrometer NEAT at the HMI in Berlin. This instrument has a much lower resolution (HWHM ≈ 35meV) than IN13 (HWHM ≈ 8meV) providing information over a wider dynamical range. The analysis of the quasi elastic spectra are now under process and will be here discussed.

Lipid/Polysaccharide Nanovectors For Drug Delivery

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In health care and pharmaceutical sciences, nanotechnologies have been indicated as a very promising field for breakthrough technological innovation in early disease diagnosis and in improved therapies. In recent years, nanotechnologies have been applied to improve drug delivery: specific nano-vectors able to carry the biologically active principle have been developed, in order to protect the encapsulated drug and to modify the kinetic of its delivery[1-3].

We have investigated the structure and morphology of self-organised lipid/saccharide nanoparticles of interest as drug vectors[4-6]. The nanoparticles were prepared by rapid injection, under mechanical stirring, of an ethanol solution of soybean lecithin into a chitosan aqueous one; nanoparticle supramolecular self-organization is driven by the interaction of negative lipid material in presence of the positively charged polysaccharide. A detailed knowledge of the nanoparticle structure as a function of chitosan content is important in order to optimize the loading efficiency and to tailor the kinetics of drug release. Lecithin is a mixture of different phospholipids and fatty acids the nanoparticle complexity, at the molecular level, is therefore high. In spite of that, we show that, by applying complementary advanced microscopic techniques (DLS, cTEM, SAXS and SANS), it is possible to describe with satisfactory detail the particle structure and morphology. The investigated nanoparticles are characterised by a hollow core (typical size ~ 700 Å), occupied by the aqueous solvent, surrounded by a multilayer structure made up by lipid bilayers each surrounded by a region containing water and chitosan. The overall particle size ranges from 800 Å to ~ 1440 Å depending on the number of bilayers in the multilayer structure. Slower kinetics of drug release are obtained using nanoparticles with a high content of multi-lamellar structures.

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Vibrational density of states in densified GeO_2 glasses

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Amorphous materials have a peculiar anomaly with respect to their crystalline counterpart, the so-called Boson Peak (BP) in the low energy phonon density of states (DoS). Density variation induces dramatic changes in the vibrational DoS so that it seems an appropriate parameter for testing the different theoretical scenarios that have been proposed in order to explain the nature of the BP. We performed an optical and spectroscopic characterization of permanently densified GeO_2 glasses, which were retrieved from various high pressures in the range from 0 to 6 Gpa.
Combining refraction index measurement and Brillouin light scattering we measured the longitudinal and transverse sound velocities and consequently the Debye energies for all the samples. Moreover ultrasonic sound attenuation measurement were carried out. This allows us to study the elastic properties evolution of the system as a function of its increasing density.
Regarding the DoS, the variations of the BP intensity and its frequency shift were studied by means of Raman and Inelastic Neutron Scattering. The obtained results confirm that the intensity of the BP decreases upon increasing the density while its position shifts to higher frequencies [2]. Scaling the abscissa, the spectra of densified samples rescale one on the other, proving the existence of a master curve [3]. Moreover, the elastic medium modification cannot fully explain the DoS evolution.

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Lysozyme in water-ethanol mixtures: preferential hydration and consequent unexpected phenomena

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In the topic of protein solvation, a quantitative estimation of the solvation shell thickness and its chemical composition was obtained by in-solution Small Angle Neutron Scattering (SANS) experiments analyzed with a global-fit approach [1-3]. In those beginning studies, two well-known cosolvents, glycerol and urea, were taken into consideration, while here we present a set of SANS experiments of lysozyme dissolved in water-ethanol mixtures. This case is more interesting, since unexpected phenomena, such us gelification and small amyloidogenic oligomers formation, occur in experimental conditions quite different from those investigated in literature [4]. We propose the protein solvation features to be strictly connected with arising of these processes.

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QENS measurements on AOT- water- decane microemulsion.

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We report results of quasi-elastic neutron scattering experiments on an inverted microemulsion system, composed of water, decane and AOT, a surfactant molecule with two

hydrophobic tails and one hydrophilic head. These last ones aggregate together to avoid the oil phase, forming spherical micelles containing a water core of which the diameter is determined by the molar ratio X=[water]/[AOT].

For X=40.8 the droplets have a radius of 5 nm and the system presents a big variety of structures, like bicontinuous, lamellar phase and oil in water microemulsions. In particular, a percolation transition is characterised on a wide range of dispersed phase f (given by the volume ratio between water+AOT and total volume), above which the short range interaction between droplets leads to a static aggregation, while below the threshold a dynamical percolation is

observed. The transition has a striking effect on the electrical conductivity, that increases by 5 order of magnitudes in crossing the percolation line[1].

The QENS measurements were performed as a function of temperature with a water-to-AOT ratio X=40.8 and a volume fraction f=0.50 around the percolation threshold.

Measurements have been carried out on protonated system and on partially deuterated samples (d-decane and D2O), in order to focus on different parts of the confined water dynamics.

Preliminary results show that the translational motion of water confined in the droplet is faster than water in bulk[2].

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POSTER

Metamagnetic transition in the eutectic system $Sr_3Ru_2O_7$–$Sr_4Ru_3O_{10}$

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The members of the Ruddlesden-Popper series with general formula $Sr_{n+1}Ru_nO_{3n+1}$ display a remarquable variety of exotic ground states. Pseudo-cubic $SrRuO_3$ is a rare example of an itinerant ferromagnet based on 4d electrons and has a Curie temperature of 160K. Two dimensional Sr_2RuO_4 is a paramagnet and, below 1.5K, a superconductor of an unconventional p-wave triplet type. $Sr_3Ru_2O_7$ is also two-dimensional, yet has not shown any superconductivity down to 400mK, even though the level of purity in floating-zone crystals is comparable with that of superconducting Sr_2RuO_4 samples. The susceptibility of $Sr_3Ru_2O_7$ shows a peak at ~16K, reminiscent of an antiferromagnetic transition. However neutron powder diffraction measurements show no sign of antiferromagnetic order down to 2K [1]. Single crystal diffraction confirms this result down to 40 mK [2]. The magnetic behaviour of the third RP series member (n=3) $Sr_4Ru_3O_{10}$ is not fully understood. Several magnetization studies of $Sr_4Ru_3O_{10}$ provide evidence for anisotropic ferromagnetism with T_{curie}=105K [3,4]. Recent neutron scattering measurements [3] have shown a ferromagnetic transition at T_{curie}=100 K with an easy axis lying in the *a-b* plane. At the same time, the recent discovery of the superconductivity at 3 K in eutectic crystals [5] of Sr_2RuO_4-Ru metal has stimulated interest in other eutectic crystals, e.g., Sr_2RuO_4-$Sr_3Ru_2O_7$ [6]. In this eutectic the magnetic and superconducting properties appear to be different from the single phase one. We have successfully grown lamellar eutectic crystals of $Sr_3Ru_2O_7$-$Sr_4Ru_3O_{10}$ in a double-mirror optical floating zone furnace [7] with different concentrations of the two phases. The eutectic dark-brown crystals grow in the [001] direction and cleave along the [110] direction as do the single phase crystals. Polarized light optical microscopy shows a clear lamellar pattern with a period of about 30 mm. XRD analysis indicate that the $Sr_3Ru_2O_7$ and $Sr_4Ru_3O_{10}$ phases match on the same crystal with parallel in-plane and out-of-plane lattice parameters. Our eutectic crystals are therefore natural junctions of the $Sr_3Ru_2O_7$ metamagnet and the $Sr_4Ru_3O_{10}$ ferromagnet and may be useful in studies of possible novel quantum critical phenomena specific to itinerant systems.

In particular, macroscopic magnetization measurements on eutectic samples of $Sr_3Ru_2O_7$-$Sr_4Ru_3O_{10}$ show a metamagnetic transition at about 3 T for a magnetic field applied in the *a-b* plane. The metamagnetic field is intermediate between that which is observed in $Sr_3Ru_2O_7$ (~5.5 tesla) and that observed in $Sr_4Ru_3O_{10}$, (~2 tesla).

In an attempt to understand the metamagnetic transition in the $Sr_3Ru_2O_7$/ $Sr_4Ru_3O_{10}$ eutectic system at a microscopic level, we have performed neutron diffraction measurements on the 4-circle diffractometer D10 at the Institut Laue- Langevin. Here we report the effect of temperature and applied magnetic field on the magnetic order.

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Lysozyme under pressure: incoherent elastic neutron scattering and small angle scattering studies

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Pressure is a fundamental thermodynamic variable for modifying protein stability and for defining protein conformational states [1]. Changes in protein structure in response to pressure can provide detailed insight into local volume fluctuations, such as those that lead to channel opening or ligand exchange [2].

Also pressure is an important environmental variable: some deep-sea organisms live at pressures of over 1 kbar, and space exploration will require a detailed understanding of the effects of pressure on organisms.

We present a study concerning the response of lysozyme, a model protein, to a pressure treatment. Newness of our approach is the combination of an elastic incoherent neutron scattering experiment, that provides new insights on the roto-traslational diffusion and internal motion features of lysozyme, and a small angle scattering experiment, that monitors both protein structure and protein-protein interactions in function of the increasing pressure. We found that on increasing the pressure the protein maintains its native structure, but is less mobile and partially modifies its interactions.

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Hydration Dynamics and Time Scales of Coupled Water-Protein Fluctuations

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Inelastic neutron scattering has been used to shed light on the rich dynamical interplay between the protein and its hydration water. The availability of the Maltose Binding Protein in both fully deuterated and hydrogenated form allowed us to reliably separate the contribution to the dynamics of the solvent interacting with biomolecule from the one of the hydrated biomolecule. In particular we studied the dynamical coupling between protein and hydration water by analyzing the dynamical susceptibility of the two systems over a wide energy range and across the dynamical transition temperature.

Analysis of porosity in Nickel-Titanium Shape Memory Alloys by means of ultra Small Angle Neutron Scattering

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Nickel-titanium shape memory alloy (SMA) is one of the most promising materials for different kinds of applications such as aeronautics and biomedicines due to two extraordinary mechanical properties (supere- lasticity and the shape memory effect) and to its high biocompatibility. Up to now, many porous NiTi SMAs with different pore structures have been developed by various techniques such as reactive sintering, hot isostatic pressing and self-propagating high-temperature synthesis or combustion synthesis [1,2]. These techniques allow reducing production time and cost compared to the melting process. However, process- ing conditions need to be controlled to obtain a homogeneous microstructure. It has been shown that the mean pore size as well as pore size distribution can be affected by electric and magnetic fields: in fact the application of electromagnetic fields to metallic materials can lead to a change of the material's structure, retardation of grain growth, reduction in cavitation, increase in width of the dispersoid-free zone adjacent to the grain boundaries and a change in its chemical composition, migration of inhomogenities and defects, their reordering and annihilation. In this study we show how ultra Small Angle Neutron Scattering analy- sis, together with Micro Computed Tomography [3], can quantitatively describe porosity of NiTi fabricated by two different advanced and low-cost techniques - Reaction Synthesis and Mechanical Alloying and Hot Pressing.

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Anomalous phase behaviour of glycolipid selfassembly tuned by sugar headgroup surface arrangement.

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We present SANS results on a family of membrane glycolipid bearing large headgroups: the gangliosides. They present an anomalous mesophase behavior, consisting in that the aggregation number of amphiphile aggregates decreases with concentration. On the contrary the conventional picture of interacting micelles says that a reduction in the molecular surface area (increase of aggregate size) is paid to reduce intermicellar interactions when the solution is concentrated. The anomalous micellar size reduction suddenly takes place at intermediate concentrations, close to phase boundary between the disordered and the ordered micellar regimes. Different glycolipids present different phenomenology. The common point at the base of this rich phenomenology is that the amphiphilic surfaces made of bulky headgroups of more or less complex sugar chains, is able to modify molecular surface area and protrusion from the aggregate, contributing to the energy balance between inter- and intra-aggregate interaction. The micellar size behaviour is observed through the analysis of the particle form factor and of the solution structure factor as obtained by SANS. A significant help in data analysis is provided by comparison with SAXS spectra on the same systems

Hydration dependent dynamics in sol–gel encapsulated myoglobin

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In this work we study the effect of hydration on the dynamics of a protein in confined geometry, i.e. encapsulated in a porous silica matrix. Using elastic neutron scattering we investigate the temperature dependence of the mean square displacements of non-exchangeable hydrogen atoms of sol–gel encapsulated met-myoglobin.

The study is extended to samples at 0.2, 0.3 and 0.5 g water/g protein fractions and comparison is made with met-myoglobin powders at the same average hydration and with a dry powder sample. Elastic data are analyzed using a model of dynamical heterogeneity to take into account deviations of elastic intensity from gaussian behavior in a large momentum transfer range and reveal a specific, model independent, effect of sol–gel confinement on protein dynamics, consisting mainly in a reduction of large scale motions that are activated at temperatures larger than 230 K. Surprisingly, the effect of confinement depends markedly on hydration and has a maximum at about 35% water/protein fraction corresponding to full first shell hydration. The presence of hydration-dependent MSD also in encapsulated met-Mb strongly supports the idea that the effect of sol–gel confinement on protein dynamics involves a modification of the structural/dynamical properties of the co-encapsulated solvent more than direct protein–matrix interactions.

Determination of the best experimental conditions to investigate macromolecule-solvent interface via in solution Small Angle Scattering experiments

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Many efforts were made in order to obtain quantitative information about protein solvation shell composition in water mixtures by a variety of thermodynamic techniques, such as dialysis equilibrium or vapor pressure osmometry. The main advantage of the use of Small Angle Scattering (SAS) techniques is the possibility to perform the experiments in an environment quite similar to that in vivo. In fact the SAS experiments concern proteins dissolved in solution, at various protein concentration values and in buffer conditions approaching the cellular environment, while the cited thermodynamic techniques should be applied at infinite protein dilution. In addition, Small Angle Scattering approach enables the simultaneous investigation of protein solvation shell composition and of protein-protein interactions and/or aggregation phenomena that may be modified by the presence of particular solutes or cosolvents.

The aim of this work is to resume how it is possible to determine protein solvation shell composition by means of a methodology based on SAS experiments and on a global-fit approach [1, 2]. It is well known that SAS is a low resolution technique and it has been already shown that to extimate the density of water in the first hydration shell is necessary to analyse with a proper model the whole scattering curves [3]. In the past years we applied a big effort to set a methodolgy that can be extensively used to investigate protein solvation features. The simple basic idea is that, because the low resolution of SAS technique, the simultaneous analysis or global-fitting of a group of curves, is undoubtely more informative than the analysis of a single curve, and of the same analysis repeated on different curves, too. The global-fit needs a model able to correlate together different experimental curves. The use of Schellman thermodynamicmodel [4] allowed to correlate together the quantity of cosolvent next to protein surface in samples prepared with different values of protein concentration and with different amounts of cosolvent. This is why now we report about the simulation methodology used to asses the best experimental conditions (sample preparation), that on the basis of the interesting protein and cosolvent, can help the experimentalist to choose the set of samples to be analyzed during the finite time available at synchrotron or neutron facilities.

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