Abstract Listing

Use your browser's Print button, or File-Print command sequence.

530356: Effects of guanidine hydrochloride on the structure and properties of beta-casein in solution and at interface with air

PHYS 0 [530356]: Effects of guanidine hydrochloride on the structure and properties of beta-casein in solution and at interface with air

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and association of biomolecules in solution*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *Y*
Special Equipment Needs: *overhead projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

We have examined the small-angle neutron scattering (SANS) profile of beta-casein in the native state and in highly denaturing conditions. It shows that the neutron spectra given by unfolded beta-casein are similar to those of excluded volume polymer chains. Adsorption layers of beta-casein formed from a buffer including various concentrations of guanidine hydrochloride (gdmCl) have been studied by neutron reflectivity. A transition in the structure and in the properties of the adsorption layer seems to occur around a gdmCl concentration of 1.5 M. These data are interpreted assuming that the adsorbed protein molecules behave like multi-block copolymers with alternating hydrophilic and hydrophobic sequences.

530380: Hydrogen and hydration in proteins

PHYS 0 [530380]: Hydrogen and hydration in proteins

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ACCEPTED

Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: High-resolution protein crystallography*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *overhead projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

One of the most important fields today is structural genomics, in which the functions of proteins are analyzed using the results from synchrotron X-ray and NMR protein structure analysis. However, it is difficult in an NMR or X-ray crystallographic analysis of a protein to identify all of the hydrogen atoms and the water molecules of hydration, even though they play important roles in innumerable biological processes. In contrast, the neutron diffraction method has the ability to locate hydrogen position absolutely. We have recently developed a neutron imaging plate (NIP) and a neutron monochromator, and have successfully applied them to construct a neutron diffractometer dedicated for biological macromolecules (BIX-3) in the JRR-3M reactor. The performance of BIX-3 has been certified as one of the best in the world. By using BIX-3, all the hydrogen atoms and most of the solvent molecules of hydration of lysozyme (Hen Egg-white L. at different pH, Human L.), myoglobin and rubredoxin (wild type and mutant), which are small but fundamentally important proteins, have been unambiguously identified in 1.5 resolution. These structural results have provided new and important discoveries such as the bifurcated hydrogen bonds in a-helices, the fine structure of methyl group, details of hydrogen/deuterium exchange reactions and the dynamic behavior of hydration in proteins. We have just finished constructing a much higher-performance neutron diffractometer for protein crystallography and this will be applied for the study of the hydration structure of DNA, and the structures of proteins complexed to pharmaceutically active molecules. The start of this new neutron structural biology project, which will use the next generation neutron source generated by a high intensity proton accelerator in the States and Japan, is also coming into view.

530424: Role of conformational dynamics for thermal adaptation of proteins

PHYS 0 [530424]: Role of conformational dynamics for thermal adaptation of proteins

Joerg Fitter, IBI-2: Structural Biology, Research Center Juelich, Juelich D-52425, Germany, Fax: +49 2461 612020, j.fitter@fz-juelich.de

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics I*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
Thermal equilibrium fluctuations play a crucial role for the balanced interplay between structural flexibility and rigidity of protein structures. A promising approach to understand the molecular mechanisms of thermal adaptation in biology is to investigate dynamical properties of proteins from mesophilic and thermophilic organisms. We study this subject for a pair of alpha-amylases with respect to dynamical, functional and thermodynamical properties (Fitter et al. Biochemistry 40, 10723, 2001). Detailed information on fluctuations on different time scales and with spatial resolution is required to distinguish between internal fluctuations essential for enzymatic activity and those contributing to the conformational entropy. The use of neutron spectroscopy measuring the internal picosecond fluctuations has demonstrated to be a very powerful approach to measure directly conformational entropy in proteins (Fitter et al. Physica B, 307,1, 2001). Recent results of neutron spectroscopy studies on alpha-amylase in the folded and the unfolded state will be presented.

530678: Thermal neutron holography, small-angle neutron scattering and biomaterials

PHYS 0 [530678]: Thermal neutron holography, small-angle neutron scattering and biomaterials

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems II*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
Biomolecules such as lipids are of great scientific interest for various and often very different reasons. For example, lipids are a major component of biological cell membranes and as a result, much effort has been expended in understanding their structure and function. On the other hand, lipids are lyotropic liquid crystals which exhibit a variety of interesting structures (e.g., lamellar, hexagonal, cubic, etc.) and serve as prototype models for certain 1D and 2D phase transitions.

Using neutrons, we have recently looked at the recently popular "bicelle" (bilayered micelles) system and have discovered that, under certain conditions bicelles transform into stable, monodisperse unilamellar vesicles suitable for drug delivery. Moreover, they can self-assemble into ribbons, a phase previously observed only in surfactant systems. Results of our most recent observations will be presented and discussed. Finally, I will introduce the newly developed technique of neutron holography which offers great promise in elucidating the three-dimensional structure of biological quasi-crystals.

530872: Neutron Interferometry of Vectorially-Oriented Single Monolayers of Membrane Proteins & Their Artificial Synthetic Maquettes

PHYS 0 [530872]: Neutron Interferometry of Vectorially-Oriented Single Monolayers of Membrane Proteins & Their Artificial Synthetic Maquettes

J. Kent Blasie[1], Larry R. Kneller[2], and Charles F. Majkrzak[2]. (1) Department of Chemistry, University of Pennsylvania, 3301 Spruce Street, Philadelphia, PA 19104-6323, Fax: 215-573-2112, jkblasie@sas.upenn.edu, (2) Center for Neutron Research, National Institute of Standards & Technology

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems II*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *PowerPoint presentation from laptop possible???*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

We wish to determine the roles of structure and conformational change in the mechanism of energy-dependent transmembrane transport of electrons and ions by membrane proteins and their models, or "maquettes". Synchrotron x-ray interferometry is employed in time-resolved structural studies of the proteins and their "maquettes" in the form of vectorially-oriented single monolayers. The single monolayers are membrane-like allowing for control of the kinetics of the chemical reactions involved in the transport process through the applied transmonolayer potential. This permits extending the lifetimes of the various chemical intermediates in the transport processes to time-frames sufficient for the collection of accurate data accumulated in serial time-frames of this duration. The structural data obtained from single monolayers of the proteins or "maquettes" can approach near atomic-resolution in the profile structure of the monolayer, the direction of net electron or ion transport. Neutron interferometry plays a key role in providing this structural information.

531291: What really drives the hydrophobic interaction?

PHYS 0 [531291]: What really drives the hydrophobic interaction?

John L. Finney, Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT, London, United Kingdom, Fax: +44 20 7679 1360, j.finney@ucl.ac.uk, Daniel T. Bowron, ISIS Facility, Rutherford Appleton Laboratory, A.K. Soper, ISIS Facility, Rutherford Appleton Laboratory, and Sanhita S. Dixit, Department of Physics and Astronomy, University of California at Los Angeles

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structural*

and dynamical aspects of biomolecular hydration
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
The hydrophobic interaction is thought to dominate many important interactions in biological systems. The conventional wisdom argues that the hydrophobic driving force relates to the 'ordering' of solvent close to a non-polar group. On bringing together two such groups in aqueous solution, 'ordered' solvent is released to the bulk solvent with a consequent gain in entropy. However, no direct experimental evidence is available to verify this view. Using neutron scattering with isotope substitution, we can obtain essentially full structural information - the partial radial distribution functions - for aqueous solutions of molecules whose interactions are driven by the hydrophobic effect. Using recent results on amphiphile solutions, we find that the experimental evidence does not support the classical view. Alternative explanations are discussed that are consistent with the experimental structural data.

532760: How does protein affect water?

PHYS 0 [532760]: How does protein affect water?

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structural and dynamical aspects of biomolecular hydration*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *Beamer*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
Characterization of the physical properties of protein surface hydration water is critical for understanding protein structure and folding. Here, using molecular dynamics simulation, we provide an explanation of recent X-ray and neutron solution scattering data that indicate that the density of water on the surface of lysozyme is significantly higher than that of bulk water. The simulation-derived scattering profiles are in excellent agreement with experiment. In the simulation the 3A-thick first hydration layer is 15% denser than bulk water. About two-thirds of this increase is due to a geometric contribution that would also be present if the water were unperturbed from the bulk. The remaining third arises from modification of the water structure and dynamics, involving approximately equal contributions from shortening of the average water-water O...O distance and an increase in the coordination number. Variation in the first hydration shell density is shown to be determined by electrostatic properties of the

protein surface and local surface topography. On average, denser water is found in depressions on the surface in which the water dipoles tend to be aligned parallel to each other by the electrostatic field generated by the protein atoms.

534141: Slow Relaxation in DNA and Proteins: A Key to the Dynamic Transition

PHYS 0 [534141]: Slow Relaxation in DNA and Proteins: A Key to the Dynamic Transition

Alexei Sokolov, Department of Polymer Science, The University of Akron, 170 University Avenue, Akron, OH 44325-3909, Fax: 330-972-5290, sokolov@polymer.uakron.edu

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics I*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

Hydrated biopolymers demonstrate dynamic transition at temperatures Td~200-230K. It shows up as a sharp rise of mean-squared atomic displacement above these temperatures. It is known that one can shift Td by placing proteins in different solutions. We analyzed dynamics of Lysozyme and DNA [1] in different solvent conditions. The results demonstrate that the dynamic transition is related to a slow relaxation process (conformational averaging) in biopolymers. Microscopic nature of the slow process and its relation to protein functions are discussed. Important observation is a correlation between Td and the crossover temperature Tc in dynamics of the solvent. These results support the idea that biopolymers are "slaves" of a solvent and that the latter controls the dynamic transition. Speculations about the nature of the dynamic transition are presented. 1. A. P. Sokolov, H. Grimm, A. Kisliuk, A.J. Dianoux, J.Biological Phys. 27, 313 (2001).

536742: Structural Biology with Spallation Neutrons

PHYS 0 [536742]: Structural Biology with Spallation Neutrons

Benno P Schoenborn, and Paul Langan, Biosciences, Los Alamos National Laboratory, M888, Los Alamos, NM 87545, schoenborn@lanl.gov

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: High-resolution protein crystallography*
Invited: *Y*
Preferred Presentation Format: *OralOnly*

Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

Data will be presented on the performance of a new neutron station for structural biology. The instrument was designed and built to optimize data collection from proteins, membranes, viruses and oriented fibre samples adapted to the characteristics of the Los Alamos Spallation Neutron Source (LANSCE). The station uses a partially decoupled Moderator and a large 2 dimensional position sensitive detector. The detector is cylindrical covering 120 degrees with a height of 20 cm. The total counting rate is over one million neutrons per second with a resolution of 1.6 mm (FWHH). Data is collected between 1 and 5 Angstroms in 96 time slices from a 20 Hertz source with the detector located at 28 meters for good wavelenght resolution. Data is therefore collected as wavelength resolved Laue data.

537296: Dynamic behavior of several cytochrome c structural states

PHYS 0 [537296]: Dynamic behavior of several cytochrome c structural states

Adam M Pivovar, NIST Center for Neutron Research, National Institute of Standards and Technology, 100 Bureau Drive Stop 8562, Gaithersburg, MD 20899-8562, Fax: 301-975-9847, adam.pivovar@nist.gov, and Mounir Tarek, Laboratoire de Chimie Theorique, Universite Henri Poincare

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics I*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

In order to deepen our understanding of the molecular motions involved in protein folding, we have employed differential quasielastic neutron scattering (QENS) to measure the dynamics of cytochrome c in the native and several unfolded states at picosecond timescales. In a typical QENS experiment, neutrons exchange both energy and momentum with the sample, allowing one to surmise the characteristic time scale and length scale, respectively, of the molecular motions involved. Another fundamental property of incoherent neutron scattering is the extremely large relative scattering cross section of hydrogen relative to all other atomic species, that is, atoms other than hydrogen remain virtually invisible in the scattering process. Because the hydrogen distribution within a protein is nearly homogeneous, an incoherent QENS experiment reflects the ensemble dynamics of the protein, particularly motions of the non-exchangeable protons of the side chains. Cytochrome c is ideally suited for these preliminary investigations as it has several well characterized and easily accessible non-native folded states that, in comparison with the native state, permit rationalization of the dynamic behavior.

The experimental results are interpreted using a model that allows one to extract an effective diffusion coefficient, determine the timescale of side chain motions and surmise the apparent geometry of these motions.

537410: Simulation, neutron, and x-ray scattering experiments for pure liquid water

PHYS 0 [537410]: Simulation, neutron, and x-ray scattering experiments for pure liquid water

Teresa Head-Gordon[1], Greg L.B. Hura[2], Robert M. Glaeser[3], and Daniela Russo[1]. (1) Department of Bioengineering, University of California, Berkeley, Berkeley, CA 94720, Fax: 510-486-6488, TLHead-Gordon@lbl.gov, (2) Biophysics Group, University of California, Berkeley, (3) Molecular and Cell Biology, University of California, Berkeley

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structural and dynamical aspects of biomolecular hydration*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *pc projector for powerpoint*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

We consider the progress of the experimental scattering and water simulation fields in obtaining reliable structural descriptions of liquid water over large regions of the phase diagram. We describe the intricate process of acquiring, processing, and correcting scattering intensity data through to the extraction of the partial radial distributions functions of water, that impact the reliability and accuracy of x-ray and neutron scattering experiments. We also consider the progress in the modeling of water using classical models and simulation methods, their improvements by incorporation of many-bodied effects through polarization, and quantum mechanical simulations that explicitly describe the electronic structure of water in the condensed phase. These complementary techniques of experimental scattering and simulation show that definitive progress is being made in the structural characterization of the topology of the hydrogen-bonded network of the water liquid.

537606: Inelastic and quasielastic neutron scattering studies on protein dynamics

PHYS 0 [537606]: Inelastic and quasielastic neutron scattering studies on protein dynamics

Mikio Kataoka, Department of Materials Science, Nara Institute of Science and Technology, Takayama, Ikoma, Japan, Fax: 81-743-72-6109, kataoka@ms.aist-nara.ac.jp

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics II*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *overhead projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

Using Staphylococcal nuclease (SNase), we have been investigating the protein dynamics with inelastic and quasielastic neutron scattering over a wide range of frequency. In order to reveal the dynamical properties specific to the folded protein, inelastic neutron scattering measurements were performed for the folded and the unfolded SNase at 100K and 300K. There are no significant differences in INS spectra between the folded and unfolded form at 100K. The spectrum can be explained qualitatively by a normal mode calculation. The changes in dynamical properties upon folding were observed at 300K in the Q-dependence of EISF, indicating that unfolding leads to an increase in the amplitude of the local internal motions. The observed EISF can be explained with diffusive motion restricted in a sphere and a jump motion between two sites. We also estimated the heterogeneity of dynamics from the Q-dependence of incoherent elastic scattering, which will be also discussed.

537679: Protein dynamics studied by neutron scattering and MD simulation

PHYS 0 [537679]: Protein dynamics studied by neutron scattering and MD simulation

Marie-Claire Bellissent-Funel, CEA-Saclay, Laboratoire Léon Brillouin (CEA-CNRS), 91191-GIF-sur-YVETTE Cedex, France, Fax: 33-1-6933-1487, mcbel@llb.saclay.cea.fr

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics II*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

It is known that water plays a major role in the stability and catalytic function of proteins. Both the effect of hydration water on the dynamics of proteins and the effect of proteins on the dynamics of water have been studied using inelastic neutron scattering. In order to characterise diffusive motions in C-phycocyanin protein neutron scattering experiments have been performed at the Laboratoire Léon Brillouin. Molecular dynamics simulation and analytical theory have been combined to analyse the data and get a detailed description of diffusive motions, respectively for hydration water and protein. The

simulation-derived dynamic structure factors are in good agreement with experiment. The dynamical parameters are shown to present a smooth variation with distance from the core of the protein. Finally, the retardation of hydration water motions is discussed in light of some model of alpha relaxation familiar in the theory of kinetic glass transition in dense supercooled liquids.

537905: Low Frequency Vibrational Modes in Plastocyanin: MD and Neutron Scattering

PHYS 0 [537905]: Low Frequency Vibrational Modes in Plastocyanin: MD and Neutron Scattering

Salvatore Cannistraro, Unità INFM, Dipartimento di Scienze Ambientali, University of Tuscia, Viterbo, Italy, Fax: 00390761357179, cannistr@unitus.it, and Anna Rita Bizzarri, Unità INFM, Dipartimento di Scienze Ambientali, University of Tuscia, Italy

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics II*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

The low-frequency dynamics of plastocyanin (PC), an electron transfer copper protein, has been investigated by incoherent neutron scattering at different temperatures and H/D exchanging conditions. The dynamic structure factor of a hydrated PC with all the exchangeable hydrogens replaced by deuterium exhibits an excess of vibrational modes at about 3.5 meV, reminiscent of the boson peak found in other proteins and glassy systems (even hydration water).When only fast exchangeable hydrogens are substituted by deuterium, PC, besides the peak at 3.5 meV, shows an additional peak at about 1 meV. These vibrational peaks are discussed in connection with the topological disorder of the systems, the fluctuations of the hydrogen bonds and Molecular Dynamics simulation results on the same system. The latter results, which refer to essentially single molecule configuration, have been able to reproduce only the 1meV peak .

538387: High Frequency Motions In Systems of Biological Interest

PHYS 0 [538387]: High Frequency Motions In Systems of Biological Interest

Mark Johnson, and Marie Plazanet, Scientific Computing, Institut Laue Langevin, 6 Rue Jules Horowitz, BP 156, Grenoble 38042, France, Fax: 33 4 76 20 76 48, johnson@ill.fr

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and*

nucleic acid dynamics I
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
Solid-like behaviour is known to play an important role in biological systems. For example, vibrational modes provide efficient contributions to structural reorganisation and energy transfer accompanying the function of a protein. The goal of our work is to characterise vibrational dynamics in bio-molecular fragments and thereby gain insight into their role in biological function. Density functional theory (DFT) based computational codes allow accurate, parameter-free calculations to be performed on molecular systems containing hundreds of atoms. Periodic boundary conditions allow crystalline solids or model structures with local order to be investigated. The inelastic neutron scattering spectrum is calculated from the normal mode frequencies and eigenvectors and can be compared directly with measured spectra, enabling computational methods to be validated. Studies on small molecule systems with extended hydrogen bond networks (DNA bases and nucleosides, molecules containing peptide groups) demonstrate how well DFT describes intra and inter molecular interactions and allows a clear understanding of the vibrational dynamics of these systems. Current work concerns hydrogen-bonded crystalline polypeptides, polyglycine and Kevlar (which exists as oriented fibres), and we intend to move on to Collagen-like systems.

538571: Probing the Dynamical Transition of Proteins: Surface-coupled and intramolecular motions

PHYS 0 [538571]: Probing the Dynamical Transition of Proteins: Surface-coupled and intramolecular motions

Wolfgang Doster, Physics Department E 13, Technical University of Munich, James Franckstrasse, Garching D-85748, Germany, Fax: 49-89-289-12473, wdoster@ph.tum.de

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics I*
Invited: *Y*
Preferred Presentation Format: *PosterOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
The question whether molecular motions contribute to enzyme activity is of considerable mechanistic interest. A straightforward approach would be to switch off particular classes of motions while recording the resulting effect on protein function. The dynamical transition in proteins leads to a drastic slowing down of solvent-coupled structural fluctuations while fast intra-molecular displacements are not

affected. The transition is driven by a diverging solvent viscosity near a liquid to glass transition, dehydration or dehydration by freezing of the solvent. Whenever the time scale of structural motions falls out of the experimentally accessible window, an elastic spectral component evolves. To establish sound dynamic correlations requires to resolve the elementary steps of enzyme kinetics and their relation to structural mobility. In this contribution the molecular mechanism of the dynamical transition in proteins, its dependence on solvent conditions, intra-molecular motions, and the related kinetic effects is addressed.Using a combination of neutron scattering, Mößbauer spectroscopy and flash photolysis experiments with myoglobin we argue that the onset of the dynamical transition and the ligand escape rate shift in phase with the solvent viscosity on protein surface. Fast intra-molecular steps such as dihedral transition or methyl group rotations are not affected by the solvent. Thus myoglobin can perform its biological function even below the dynamical transition temperature but with slow pace.

538881: Correlated protein dynamics at 1.1 Å resolution by neutron diffraction

PHYS 0 [538881]: Correlated protein dynamics at 1.1 Å resolution by neutron diffraction

Martha M. Teeter, Department of Chemistry, Boston College/UC Davis, 140 Commonwealth Ave., Chestnut Hill, MA 02467, Fax: 530-752-8995, teeter@bc.edu

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: High-resolution protein crystallography*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *overhead backup for computer projection*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

Neutron diffraction data from 1 mm^3 crystals of the small hydrophobic protein crambin (4.7 kDa, 46 residues) were collected with 1.1 Å radiation on the HFBR at Brookhaven National Laboratory using a He3 detector. The structure was refined with the programs PROLSQ, SHELX93, and SHELX97. The crystals contain primarily the Pro22/Leu25 sequence isomer of crambin and the results are compared to the X-ray structure of Pro/Leu crambin (A. Yamano & M.M. Teeter. (1994) J. Biol. Chem., 269, 13956-13965.)

The structure reveals correlated multiple substates (discrete disorder) of protein side chains. A pentagonal water ring around Leu18 shows discrete hydrogen-bonding disorder in both the protein and solvent regions particularly clearly. Such hydrogen-bonding disorder is correlated to the protein atom donor or acceptor character or both (for hydroxyl). Certain solvent atoms reveal more dynamic character of water due to imbalances between the donors and acceptors at the protein surface.

538956: Structure and Function of Biological Macromolecules in Solution: SANS Data Analysis and Modeling Methods

PHYS 0 [538956]: Structure and Function of Biological Macromolecules in Solution: SANS Data Analysis and Modeling Methods

Susan K. Gregurick, Department of Chemistry and Biochemistry, University of Maryland, Baltimore County (UMBC), 1000 Hilltop Circle, Baltimore, MD 21250, Fax: 410-455-2608, greguric@research.umbc.edu

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and association of biomolecules in solution*
Invited: *Y*
Comments to Organizer: *Susan Krueger and Susan Gregurick talks back-to-back,please*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *I will give a powerpoint talk, and I will bring a PC but not projector*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

Within the past decade, small angle scattering measurements (SANS and SAXS) have played an important role in molecular biology, including the studies of protein-DNA interactions, protein-protein interactions, domain interactions within a given protein and the study of nucleic acid structures (DNA, RNA and peptide nucleic acids, or PNA). The versatility of small angle scattering measurements is due, in part, to the range of length scales probed, from 10 to 1,000 Å. In order to model a three-dimensional macromolecule structure from an experimental scattering profile (I(Q) vs. Q), we have developed a series of modeling and simulation programs. Our talk will highlight three examples (1). A Monte-Carlo optimization program for the study of single and double stranded helical structures (2). An X-ray crystallographic based scattering program to simulate scattering profiles, which includes a treatment of solvation effects and (3). An illustration of the SANS data analysis and structure modeling (web-based) package.

The first part of the talk will focus on single and double stranded nucleic acid structures, such as DNA, RNA and PNA, studied over a wide range of temperatures. A Monte-Carlo optimization algorithm was developed in order to generate a best-fit double or single strand helical structure to the experimental scattering data. The versatility of such a program is that one can study helical changes over a wide range of experimental conditions. The second half of the talk will illustrate an X-ray crystallographic based method for the treatment of solvation effects in the calculation of scattering profiles (I(Q) vs. Q). Our method will be compared to the program CRYSON {Svergun, D. I., Barberato, C., and Koch, M. H. J., J.Appl. Crystallogr., 28:768-773 (1995)}. Lastly, an illustration of the entire date analysis and modeling package (web-base platform) will be demonstrated.

538960: Structure and function of biological macromolecules in solution: SANS experimental methods

PHYS 0 [538960]: Structure and function of biological macromolecules in solution: SANS experimental methods

Susan Krueger, NIST Center for Neutron Research, NIST, 100 Bureau Drive, Stop 8562, Gaithersburg, MD 20899-8562, susan.krueger@nist.gov

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and association of biomolecules in solution*
Invited: *Y*
Comments to Organizer: *Susan Krueger and Susan K. Gregurick papers should go back to back (in the order above), please! Thanks!*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Special Equipment Needs: *I can use overheads but I prefer to make a Powerpoint presentation*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

Since neutrons are sensitive to the positions of the light elements such as H, C, N and O, which are of central importance to all biological systems, small-angle neutron scattering (SANS) can provide unique information on the structure and function of biological macromolecules. Particularly powerful is the contrast variation technique, in which the isotopic substitution of D for H is routinely used to change the scattering from a macromolecule without affecting its biochemistry. The technique is extremely effective for the study of structural changes upon binding of nucleotides, lipids, peptides or cofactors, since the scattering from the newly-bound component can be separated from that of the original macromolecule. Thus, unique structural information about each component individually, as it is interacting with the other in the complex, is obtained. This talk will focus on the unique role of SANS in the study of macromolecular structure and function. The experimental methods which allow this information to be acquired will be described and examples of recent experiments will be presented.

539234: Insights into the role of solvent on the glass dynamics of proteins through the use of molecular dynamics calculations

PHYS 0 [539234]: Insights into the role of solvent on the glass dynamics of proteins through the use of molecular dynamics calculations

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics II*
Invited: *N*

Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
Over the past few decades a tremendous amount of information obtained by experimental and theoretical means has lead to our current understanding of the glass dynamics of macromolecules under various environmental conditions. In this paper we will present recent molecular dynamics simulation results obtained in an effort to determine the influence of solvent on the glass dynamics of proteins in powder, crystalline and hydrated forms. Our results will be compared to experimental incoherent neutron scattering and recent nuclear magnetic resonance relaxation measurements.

539588: Structure-dynamics-function correlation in PM

PHYS 0 [539588]: Structure-dynamics-function correlation in PM

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems I*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
The role of hydration was studied in bacteriorhodopsin (BR), the proton pump embedded in purple membrane (PM). A precise correlation between the biological functionality of BR and the structure and dynamics of hydrated PM multilayers was revealed. The hydration level of the membranes was scanned between 200 K and 300 K, including the dehydration/rehydration transition. Simultaneously the internal flexibility of PM was monitored by neutron scattering determination of amplitudes and rates of localized diffusive molecular motions and of quasi-harmonic vibrations. We show that the variation of these parameters correlates extremely well with that of the photoactivity of this system and with the layer thickness and diffusion coefficient of the liquid water on the membranes. This demonstrates the extent to which the very presence of liquid water itself and the internal mobility of PM guaranteed by it on the atomic scale, are essential for the functioning of the biological system.

540110: Structure analysis of biological macromolecules with small and medium

angle X-ray and neutron scattering

PHYS 0 [540110]: Structure analysis of biological macromolecules with small and medium angle X-ray and neutron scattering

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and association of biomolecules in solution*
Invited: *Y*
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Consider for Sci-Mix: *N*
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Abstract

Recently developed methods to analyze synchrotron X-ray and neutron scattering data from solutions of biological macromolecules are presented. These methods include: ab initio low resolution shape determination [1]; modeling of quaternary structure by rigid body refinement [2]; analysis of the medium-angle data to obtain domain structure ab initio [3]; the use of specific deuteration combined with contrast variation in neutron scattering to construct detailed inhomogeneous structural models [4]. Practical applications of these methods are illustrated by recent examples.

[1] Svergun, D.I. (1999) Biophys. J. 76, 2879-2886; [2] Kozin, M.B. & Svergun, D.I. (2000) J. Appl. Crystallogr. 33, 775-777; [3] Svergun, D.I., Petoukhov, M.V. & Koch, M.H.J. (2001) Biophys. J. 80, 2946-2953; [4] Svergun, D.I. & Nierhaus, K.H. (2000) J. Biol. Chem. 275, 14432-14439.

540206: Hydration water dynamics of an hydrophobic small oligo-peptide

PHYS 0 [540206]: Hydration water dynamics of an hydrophobic small oligo-peptide

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structural and dynamical aspects of biomolecular hydration*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
The dynamics of hydration water of a completely deuterated penta-Alanine peptide (Ala5) has been studied by inchoherent quasi-elastic neutron scattering. Measurements have been made a different levels of hydration (7%,, 30%, 50%, 90%), and on the dryed powder (0%) which is contains one structural water molecule. The dynamical contribution of this first hydration molecule of water is caracteristic of a slow rotational motion with a relaxation time of 2.2 ps. Adding two more hydration water (7%) the rotational motion of the first water is coupled with diffusive motion, and the dynamics profile can be, in first approximation, described trought a rotational jump model. At higher hydration, the mobility of the new molecules of water is quite similar to a bulk water dynamical behaviour, with a rotation relaxation time of 1 ps and a confined diffusing motion.

540226: Adsorption kinetics of phospholipid membranes to solid-liquid interfaces. Time-resolved neutron reflectivity studies

PHYS 0 [540226]: Adsorption kinetics of phospholipid membranes to solid-liquid interfaces. Time-resolved neutron reflectivity studies

Thomas Gutberlet, SF1, Hahn-Meitner-Institute Berlin, Glienicker Str. 100, Berlin 14109, Germany, Fax: 49-30-80623094, gutberlet@hmi.de, Roland Steitz, Iwan Stransky Inst, TU Berlin, Giovanna Fragneto, ILL, and Beate Kloesgen, FU Berlin

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems I*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Last Modified: *2002-04-02*

Abstract
The structure of biomimetic films along a planar surface is of interest for the construction of receptor based biosensors and as model systems for studying adsorption and interaction of biomolecules with model membranes [E. Sackmann, Science, 271, 1996, 43]. The first step for the investigation of such systems is the preparation of phospholipid molecules in the form of planar bilayers along adequate interfaces. Such oriented membranes can be obtained either by spontaneous fusion of small uni-lamellar vesicles to solid-liquid or solid-air interfaces [M. Wagner, L. Tamm, Biophys. J., 79, 2000, 1400], or by Langmuir-Blodgett techniques [T. Charitat et al., Eur. Phys. J. B, 8, 1999, 583]. The adsorption process of phospholipid molecules onto either bare or polymer coated Si-crystals is the initial subject of our studies. Neutron reflectivity was recently applied to monitor the adsorption of dimyristoyl phosphatidylcholine (DMPC) in D2O onto a planar hydrophobic polystyrene interface, deposited by spin-coating on a Si-crystal . Immediately after injection of the phospholipid vesicle suspension into the sample cell, formation of a lipid monolayer was observed in the reflectivity curve recorded. Further adsorption of an additional lipid bilayer occurred slowly in time [T. Gutberlet et al., Appl. Phys. A, 2002, accepted]. With bare planar hydrophilic Si-crystal surface, the formation of a single fluid phospholipid bilayer was monitored using time-resolved neutron reflectivity towards. Complete reflectivity curves were collected within minute time intervals at time-of-flight reflectometer D17 at

ILL. The severe but reasonable differences for the deposition of phospholipid model membranes dependent on the hydrophilicity of the layer support, a result which has to be considered for the design of model systems for studying adsorption and interaction of peptides and proteins with bilayer interfaces.

544040: Determination of dynamic 3D structures of membranes from 1D data: Molecular Dynamics/Absolute Scale Refinement (MoDAS)

PHYS 0 [544040]: Determination of dynamic 3D structures of membranes from 1D data: Molecular Dynamics/Absolute Scale Refinement (MoDAS)

Stephen H. White, Department of Physiology and Biophysics, University of California, Irvine, D334 Medical Sciences I, Irvine, CA 92697, shwhite@uci.edu, Kalina Hristova, Materials Science and Engineering, Johns Hopkins University, and Douglas J. Tobias, Department of Chemistry, University of California, Irvine

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems I*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

Combined x-ray and neutron diffraction measurements on an absolute scattering-length density scale can be used to obtain the transbilayer probability distribution functions of the principal lipid structural groups of lipid bilayers, such as the phosphate, choline, and carbonyls. But these distributions provide only a 1-D representation of bilayer structure, because they are time-averaged projections of the atomic positions onto the bilayer normal. 3-D representations of bilayer structure, on the other hand, can be obtained from molecular dynamics simulations. But these representations are tied only indirectly to experimental data. Furthermore, long simulation times are required to achieve equilibrium structures. The object of MoDAS refinement is to determine, relatively rapidly, experimentally validated dynamic 3-D structures of lipid bilayers. The method revolves around the use of restraint potentials to force the simulated bilayer to conform to the experimentally observed distributions early in the simulation period. The restraint potentials are then gradually reduced to zero in the course of the simulation so that, at equilibrium, the unconstrained bilayer dynamics underlying the experimental data can be revealed. We expect that this general approach will ultimately allow MD simulations to become a significant refinement tool for determining the structural ensembles of peptides in lipid membranes. Research supported in part by the NIH (GM46823).

544065: Neutron crystallographic studies of detergent binding in single crystals of membrane proteins

PHYS 0 [544065]: Neutron crystallographic studies of detergent binding in single crystals of membrane proteins

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: High-resolution protein crystallography*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-05-01*

Abstract

The natural environment of membrane proteins places them in contact with lipids within the membrane, water in the extra-membrane space and often with other proteins within or adjacent to the membrane. It is usually not possible to perform high resolution structural studies on these proteins in their natural environment. Instead they must be solubilised, most often in detergent, and studied for example as protein-detergent complexes in single crystals by X-ray crystallography. Up to now such studies have been successful in revealing the high resolution structure of a small number of such proteins but in no case are they able to "see" the detergent phase. This is due to the dynamic disorder and very low contrast of these molecules for X-ray diffraction. Neutron diffraction then becomes the method of choice where through exploitation of H2O/D2O exchange the contrast of the detergent may be dramatically enhanced. This allows a full structure of the protein-detergent complex to be determined; the protein with X-rays and the detergent with neutrons. Due to the disorder arising from the fluidity of the detergent phase the detergent model has only a resolution of ~10Å in the best cases. This is however sufficient to provide information on two different aspects of the structure: 1.) The nature of the protein-detergent interactions which may in some respects mimic protein-lipid interactions in vivo. 2.) The importance of different interactions in the crystal (protein-protein, protein-detergent, detergent-detergent) can be assessed and the crystallisation process eventually be better understood. The neutron low resolution crystallographic technique has been applied now to a number of membrane-protein systems. Amongst these are different forms of the protein Ompf from the outer membrane of Gram negative bacteria. The protein from E. Coli was crystallized in different crystal forms and using different detergents. The detergent binding surface is the same in each case but the crystal packing is very different. The protein from Rhodobacter capsulatus packs in yet a different way although the detergent binding surface is again very similar. Recently the detergent structure in the monomeric outer membrane phospholipase A (OMPLA) hasa also been solved (Snijder, Timmins and Dijkstra, in preparation) has also been solved and shows yet a different arrangement.

544183: Collective dynamics in lipid bilayers studied by inelastic x-ray scattering

PHYS 0 [544183]: Collective dynamics in lipid bilayers studied by inelastic x-ray scattering

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems II*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract

The short wave length density fluctuations of pure DLPC (C_{12}), DMPC (C_{14}) and DMPC with Cholesterol, bilayers close to full hydration has been studied by high-resolution inelastic x-ray scattering (IXS) technique in the gel and liquid crystal phases. The analysis based on a generalized three effective eigen-mode theory [1] allows us to construct the dispersion relation of the in-plane high frequency density oscillation modes for the first time [2]. The marked softening of the excitation near k=14 nm^{-1}, corresponding to the lipid chain-chain correlation peak in the structure factor, in the liquid crystal phase is observed. This mode of lipid chain oscillation may be of importance to transport of small molecules across membranes. The effect of added Cholesterol on the dynamics is seen to be equivalent to lowering of the effective temperature of the bilayer [4]. The generalized dynamic structure as measured by IXS and hence the dispersion relation have been calculated by a.MD simulation recently, which shows quantitative agreements with the experiment [3].

[1] C. Liao and S.H. Chen, "Theory of the generalized dynamic structure factor of supramolecular fluids measured by inelastic x-ray scattering', PRE 64, 021205(2001).

[2] S.H. Chen, C. Liao, H.W. Huang, T.M. Weiss, M.C. Bellissent-Funel and F. Sette, "Collective dynamics in fully hydrated Phospholipid bilayers studied by IXS", PRL 86, 740 (2001).

[3] M. Tarek, D.J. Tobias, S.H. Chen and M.L. Klein, "Short wavelength collective dynamics in Phospholipid bilayers: a molecular dynamics study", PRL 87, 238101 (2001).

[4] T.M. Weiss, P.J. Chen, H.W. Huang, S.H. Chen, H. Sinn and E. Alp (to be published).

544218: Microscopic views on the structure of lipid surface monolayers: the quest for surface-sensitive neutron scattering experiments

PHYS 0 [544218]: Microscopic views on the structure of lipid surface monolayers: the quest for surface-sensitive neutron scattering experiments

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ACCEPTED

Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems II*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
Nanotechnology and molecular (bio-)engineering are making ever deepening inroads into everybody's daily life. Physicochemical and biotechnological achievements in the design of physiologically active supramolecular assemblies have brought about the quest for their submolecular-level characterization. We employ surface-sensitive scattering techniques for the investigation of planar lipid membranes - for the most part, floating monolayers on aqueous surfaces - to correlate structural, functional and dynamic aspects of biomembrane models. This contribution surveys recent work on the submolecular structure of floating phospholipid surface monolayers - where the advent of third-generation synchrotron x-ray sources has driven the development of realistic, submolecular-scale chemical models [1,2] - and on the conformational control of water-soluble grafted 'polymer brushes' [3,4]. The very limited availability of neutron beamlines which enable scattering measurements from horizontal fluid surfaces has in the recent past severely impeded further development of this field. Fortunately, as prospects in this area brighten with new sources in various states of planning and commissioning worldwide, this stringent situation is expected to relax considerably. Perspectives for the life sciences and materials engineering of surface-sensitive scattering that are becoming available with state-of-the-art neutron sources will be given.

[1] M. Schalke, P. Krueger, M. Weygand, and M. Loesche, Biochim. Biophys. Acta 1464, 113 (2000).

[2] M. Weygand et al., J. Phys. Chem. B, in press (2002).

[3] E. Politsche, G. Cevc, A. Wurlitzer, and M. Loesche, Macromolecules 34, 1328 (2001).

[4] A. Wurlitzer et al., Macromolecules 34, 1334 (2001).

544232: Light-driven proton pump bacteriorhodopsin as seen by neutrons

PHYS 0 [544232]: Light-driven proton pump bacteriorhodopsin as seen by neutrons

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems I*
Invited: *Y*
Preferred Presentation Format: *OralOnly*

Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
Neutron scattering played an important role in our attempts to elucidate the mechanism of bacteriorhodopsin (bR) on the basis of its structure and dynamics. Early neutron diffraction experiments identified the location of the proton wire across bR in the projected structure of the purple membrane (Papadopoulos et al., J. Mol. Biol. 214, 15, 1990). Changes in the tertiary structure during the photocycle of bR, rising between the M1 and M2 intermediates, were first observed by neutrons (Dencher et al., Proc. Natl. Acad. Sci. U S A 86, 7876, 1989). The characteristics of thermal equilibrium fluctuations and their dependence on temperature and hydration were determined by incoherent neutron scattering (Fitter et al., Proc. Natl. Acad. Sci. USA, 93, 7600, 1996) It became evident that the large amplitudes of diffusive motions are necessary to overcome activation barriers between intermediate states. The results were directly compared to molecular dynamics simulations on bR.

544247: Neutron views of the dynamics of proteins at low temperatures

PHYS 0 [544247]: Neutron views of the dynamics of proteins at low temperatures

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ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics II*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2002-04-02*

Abstract
Much current experimental and theoretical work focuses on the way in which the dynamics of biomolecules evolves from a purely harmonic regime ($T < 50$ K) towards the rich energy land-scape at higher temperatures. Neutron data for $S_{qe}(Q;T)$, the momentum and temperature dependent integrated quasielastic intensities, are available now for nearly a dozen globular proteins. However, comparisons of the behaviour of $d(\log S_{qe})/dQ^2$ as a function of temperature reveal substantial qualitative and quantitative discrepancies that are not easily explained by structural and hydration differences of the proteins studied. It seems clear that the nonlinear mobility increases observed around and above 200 K cannot be interpreted only on the basis of a single highly averaged quantity such as $S_{qe}(Q;T)$. Information from spectrally resolved data sets, together with relevant data on (poly)peptides and on spatially resolved B-factors from low-temperature crystallography, needs to be incorporated into more sophisticated models capable of accounting for essential features of the complex picture emerging from different experimental approaches. Based on a shell model for a hydrated globular protein, this paper

describes and discusses expressions for $S_{inc}(Q,w;T)$, the temperature-dependent incoherent dynamical struc-ture factor, which go some way towards establishing a unified framework for interpretation. Neutron backscattering and time-of-flight spectra from work on globular and fibrous proteins at ISIS, ILL and PSI are used to support the model proposed.

550248: Introductory Remarks

0 [550248]: Introductory Remarks

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems I* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
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Abstract: Abstract text not available.

550249: Intermission

0 [550249]: Intermission

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems I* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2002-04-02*

Abstract: Abstract text not available.

550258: Intermission

0 [550258]: Intermission

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and dynamics of biomembranes and related systems II* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2002-04-02*

Abstract: Abstract text not available.

550259: Intermission

0 [550259]: Intermission

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics I* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2002-04-02*

Abstract: Abstract text not available.

550261: Intermission

0 [550261]: Intermission

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structural and dynamical aspects of biomolecular hydration* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2002-04-02*

Abstract: Abstract text not available.

550263: Intermission

0 [550263]: Intermission

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Structure and association of biomolecules in solution* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2002-04-02*

Abstract: Abstract text not available.

550265: Intermission

0 [550265]: Intermission

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: Protein and nucleic acid dynamics II* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2002-04-02*

Abstract: Abstract text not available.

562493: Intermission

0 [562493]: Intermission

ACCEPTED
Topic Selection: *Applications of Neutron Scattering in Structural Biology and Biophysics: High-resolution protein crystallography* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2002-05-01*

Abstract: Abstract text not available.
