Biomaterial Interfaces
Room 313 - Session BI-MoA

Biomaterials and Neutrons (BioMaN) II

Moderator: M. Grunze, Universität Heidelberg, Germany

2:00pm **BI-MoA1 Effective Protein-Protein Interaction and Clustering Phenomenon in Solution Studied by Small-Angle Neutron Scattering**, ***S.-H. Chen,*** Massachusetts Institute of Technology **INVITED**

The bottleneck of protein crystallography is the lack of systematic methods to obtain protein crystals, which is partly due to imprecise understanding of the physical chemistry conditions that control the growth of protein crystals. A general knowledge and comprehension of the effective protein-protein interaction potential in solution and the resulting phase behavior thus becomes essential. It has been shown that the crystallization curves of some globular proteins appear to coincide with the phase diagrams of a hard sphere system interacting with a short range attraction.@footnote 1,2,3@ Moreover, the study of the intensity distribution, I(Q), of some proteins measured with small angle neutron and X-ray scattering also suggests presence of a short-range attractive interaction between protein molecules besides the electrostatic repulsion induced by the residual charges in protein molecules.@footnote 4,5,6@ The so-called DLVO potential, which has been successfully applied in many colloidal systems, meets some successes when applied to protein solutions,@footnote 3,4,13@ but is still not enough to explain all the phenomena.@footnote 4,7,8,9@ Due to the complexity (anisotropic property, irregular shape, distributed charge patches, etc.), the full understanding of the properties of the effective interaction between protein molecules in solutions remains a challenge.@footnote 8@ Recent measurements of small angle neutron scattering (SANS) intensity distribution, in protein solutions by my group at MIT and others show some interesting results.@footnote 6,10,14@ First, besides the first diffraction peak, arising from the nearest neighbor inter-particle correlation in the liquid, there is an extra peak appearing at a much smaller scattering wave vector Q, due to the formation of well-ordered clusters inside the solutions. The appearance of this cluster peak is explained as due to the competition between the short-range attraction and the intermediate-range electrostatic repulsion in the effective protein-protein interaction potential in solution.@footnote 5,11,12@ Secondly, a rising intensity as Q approaching zero is observed in both liquid-like and solid-like samples, which can be shown to be due to the presence of another weak, very long-range attractive interaction term, in addition to the already proven short-range attraction and intermediate-range electrostatic HYPERLINK "mailto:repulsion.@footnote"repulsion.@footnote 12,14@ In this lecture, I shall show the results of a systematic SANS investigation of the clustering phenomenon and the newly found increasing low-Q intensity and its relation to the long-range interaction term. @FootnoteText@ @footnote 1@ D. Rosenbaum et al., Phys. Rev. Lett. 76, 150 (1996). @footnote 2@ M. H. J. Hagen et al., J. Chem. Phys. 101, 4093 (1994). @footnote 3@ G. Pellicane et al., J. Phys.: Condens. Matter 16, S4923 (2004). @footnote 4@ A. Tardieu et al., J. Cryst. Growth 196, 193 (1999). @footnote 5@ A. Stradner, et al., Nature 432, 492 (2004). @footnote 6@ B. Lonetti, E. Fratini and P. Baglioni., Phys. Chem. Chem. Phys. 6, 1388 (2004). @footnote 7@ M. L. Broide et al., Phys. Rev. E 53, 6325 (1996). @footnote 8@ R. Piazza, Curr. Opin. Colloidal Interface Sci. 8, 515 (2004). @footnote 9@ A. Striolo et al., J. Chem. Phys. 116, 7733 (2002). @footnote 10@ P. Baglioni, E. Fratini, B. Lonetti and S.H. Chen., J. Phys.: Condens. Matter 16, S5003 (2004). @footnote 11@ F. Sciortino et al., Phys. Rev. Lett. 93, 055701 (2004). @footnote 12@ Y. Liu, W.R. Chen and S.H. Chen., J. Chem. Phys. 122, 044507 (2005). @footnote 13@ C. F. Wu and S.H. Chen., J. Chem. Phys. 87, 6199, (1987). @footnote 14@ Y. Liu, E. Fratini, P. Baglioni, W.R. Chen and S.H. Chen (submitted to Phys. Rev. Lett.).

2:40pm **BI-MoA3 Small-Angle Neutron Scattering: A High Resolution, Non-Destructive Probe Of Biomacromolecular Structure**, ***O. Byron,*** University of Glasgow, UK **INVITED**

Neutrons are of particular utility in the characterisation of biomaterials because of the large difference in their interaction with the @super 1@H nucleus compared with the @super 2@H nucleus. This allows contrast variation experiments to be performed in which certain components of complex biomaterials are made to be “invisible”. In addition, neutrons do not damage biomaterials in the same way as their x-ray counterparts may do. Small-angle neutron scattering has been used to successfully reveal the molecular architecture of a range of biomaterials. I will describe its use in several systems and will include the following areas: Diblock copolypeptides constructed via designed molecular self-assembly; Nanomolecular architecture of biodegradable biopolymer inclusion bodies; Temperature response of dental-ceramics; Characterisation of medical biosurfaces resistant to biofouling

3:20pm **BI-MoA5 Determining the Structures of Peptides in Membranes Using Diffraction and MD Simulations**, ***S.H. White,*** University of California at Irvine **INVITED**

Quantitative structural images of peptides in oriented arrays of fluid lipid bilayers are necessary for interpreting thermodynamic measurements of peptide-bilayer energetics in molecular terms. Lamellar x-ray and neutron diffraction provide a starting point for obtaining structural images. But the high thermal motion of fluid bilayers limits “structures” to so-called bilayer profiles, representing a time-averaged projection of the unit-cell contents onto an axis normal to the bilayer plane. Specific deuteration of lipid structural groups combined with neutron diffraction difference methods allow these profiles to be decomposed into a collection of groups (phosphates, carbonyls, etc.) representing transbilayer probability distribution functions. The power of this method has been extended through the inclusion of x-ray data and a joint-refinement protocol. We have developed an x-ray method, referred to as absolute-scale refinement, that permits the determination of the disposition of peptides in fluid bilayers. These various approaches can used in concert as a powerful tool for gaining structural information. But that information is still only one-dimensional. We are now developing methods for obtaining experimentally validated three-dimensional structures by combining the diffraction methods with molecular dynamics simulations. In essence, our goal is to convert 1-D experimental data into 3-D images. Importantly, these images will be dynamic, which will permit the ensembles of peptide-lipid structures to be explored in detail. An essential issue, however, is the validation of MD simulations using diffraction data. A method of accomplishing this objective will be described. Research supported in part by grants from the National Institute of General Medical Sciences (GM46283 and GM68002) and the National Center for Research Resources (RR14812).

4:00pm **BI-MoA7 Exploring the Collective Dynamics of Lipid Membranes with Inelastic Neutron Scattering**, ***M.C. Rheinstädter,*** Institut Laue-Langevin, Grenoble, France **INVITED**

While most spectroscopic techniques, as e.g. nuclear magnetic resonance or dielectric spectroscopy, probe macroscopic responses, neutron and within some restrictions also x-ray scattering experiments give the unique access to microscopic dynamics at length scales of intermolecular or atomic distances. Only recently, it has become possible to study collective dynamics of planar lipid bilayers using neutron spectroscopy techniques.@footnote 1@ We determined the dispersion relation of the coherent fast picosecond density fluctuations on nearest neighbor distances of the phospholipid acyl chains in the gel and in the fluid phases of a DMPC bilayer. The experiments shed light on the evolution of structure and dynamics, and the relation between them, in the range of the gel-fluid main phase transition. The scattering volume restriction for inelastic neutron experiments was overcome by stacking several thousand highly aligned membrane bilayers. By combining different neutron scattering techniques, namely three-axis, backscattering and spin-echo spectroscopy, we present measurements of short and long wavelength collective fluctuations in biomimetic and biological membranes in a large range in momentum and energy transfer, covering time scales from about 0.1 ps to 150 ns and length scales from 3Å to about 1000 Å. A recent backscattering study gives information about slow molecular dynamics of lipid acyl chains and the 'membrane-water', i.e. the water molecules in between the stacked bilayers, in the nanosecond time range.@footnote 2@ The dispersion relations of the long wavelength undulation modes in lipid bilayers with nanosecond relaxation times can be determined by quasielastic reflectometry on spin-echo spectrometers and give direct access to the elasticity parameters of the membranes. @FootnoteText@ @footnote 1@ M.C. Rheinstädter, C. Ollinger, G. Fragneto, F. Demmel and T. Salditt, Phys. Rev. Lett. 93, 108107 (2004). @footnote 2@ Maikel C. Rheinstädter, Tilo Seydel, Franz Demmel and Tim Salditt, Phys. Rev. E, in print (2005), cond-mat/0501752.

4:40pm **BI-MoA9 Meeting the Challenges in Bio-Materials Research using Neutrons**, ***I. Anderson,*** Oak Ridge National Laboratory **INVITED**

When the Spallation Neutron Source, presently under construction in Oak Ridge, Tennessee, comes into operation in 2006 it will provide researchers across the world with unprecedented capabilities for the study of materials

using neutron beams. A comprehensive suite of instrumentation is under construction to address new challenges in a wide range of disciplines including physics, materials science, environment, nanotechnology, biology and medical sciences. An overview will be given of the range of applications and promising new areas of research relevant to Biomaterial Interfaces with emphasis on the new capabilities provided by SNS.

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