

Wednesday Afternoon, November 2, 2011

Neutron Scattering Focus Topic

Room: 207 - Session NT+AS-WeA

Applications of Neutron Scattering II

Moderator: J. Majewski, Los Alamos National Laboratory

3:00pm NT+AS-WeA4 Probing Fractals by the Combined Ultra-Small- and Small-Angle Neutron Scattering (USANS/SANS) Technique, *M. Agamalian*, Oak Ridge National Laboratory

Many natural and man-made materials exhibiting multi-level morphology (atoms – molecules – aggregates – agglomerates), in other words, existence of intermediate structural units between atomic/molecular and macroscopic levels, usually call hierarchical structures. The combined USANS/SANS is one of the best techniques using at present time for characterization of the hierarchical structures, which in many cases shows fractal behavior. The current presentation is focused at the mass and surface fractals discovered experimentally in the sedimentary rocks, attractive colloidal glasses and aggregates of soot particles in MCT-30 engine oil. Some of the fractal structures, particularly the surface fractals in rocks, are extended over three orders of magnitude in the length scale; therefore, application of the combine USANS/SANS technique, which covers the Q-range extended over five orders of magnitude in the reciprocal space ($2 \times 10^{-5} \text{ \AA}^{-1} < Q < 1 \text{ \AA}^{-1}$), is required to obtain complete structural information for complicated hierarchical structures with fractals.

4:20pm NT+AS-WeA8 Interaction of Alzheimer's Disease Tau Protein with Model Lipid Membranes, *E.M. Jones*, Univ. of New Mexico, *M. Dubey*, Los Alamos National Lab, *P.J. Camp*, *B.C. Givler*, Univ. of New Mexico, *J. Biernat*, *E. Mandelkow*, Max Planck Unit for Structural Biology, Germany, *J. Majewski*, Los Alamos National Lab, *E.Y. Chi*, Univ. of New Mexico **INVITED**

In addition to amyloid plaques, tau neurofibrillary tangles comprise another pathological hallmark of Alzheimer's disease (AD). The mechanism of tau's misfolding and aggregation is unknown, but evidence suggests that tau in AD brains may abnormally interact with the neuronal cell membrane. Using lipid monolayers at the air/water interface and supported lipid bilayers as model membrane systems, we characterized the interaction between 4 tau constructs with membranes of different lipid compositions and elucidated the structure of the protein-membrane films using a combination of biophysical techniques, including pressure-area isotherms, fluorescence microscopy, and x-ray and neutron scattering. Our data show that the full length human tau (hTau40) and its constructs are highly surface active and exhibited strong association with negative DMPG lipids and induced morphological changes observed with fluorescence microscopy, while exhibiting weaker and no interactions with positive DMTAP and neutral DMPC lipids. To elucidate molecular-scale structural details, we used X-ray scattering techniques to study tau and lipid monolayer association. X-ray reflectivity modeling indicated hTau40's presence under a DMPG monolayer and partial insertion into the lipid headgroup region, while grazing incidence X-ray diffraction data showed hTau40 insertion disrupted lipid packing. We also used neutron reflectivity assays to investigate hTau40's ability to disrupt lipid bilayers. The protein completely disrupted a DMPG bilayer while not affecting a neutral DPPC bilayer. These results indicate hTau40 has a propensity to interact with a negatively charged membrane surface and disrupt lipid packing, suggesting a possible protein-aggregate induced mechanism for aggregation and toxicity.

5:00pm NT+AS-WeA10 Stabilization of a Lipid Multilayer System by Polysaccharides, *M. Kreuzer*, *M. Strobl*, University of Heidelberg, Germany, *M. Reinhardt*, *R. Steitz*, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany, *R. Dahint*, University of Heidelberg, Germany

Hyaluronic acid (HA) is a high molecular weight polysaccharide. It is involved in a wide range of processes in the human body, such as wound healing, tumor progression and joint lubrication. Here we show that HA also stabilizes a lipid multilayer system at physiological conditions. The observed effect may be an important contribution to joint lubrication as lipid films covering the cartilage of natural joints are assumed to reduce internal friction. Neutron reflectometry investigations were carried out at V6 and the new BioRef neutron reflectometer at Helmholtz-Zentrum Berlin. Measurements against excess D₂O verified, that an oligolamellar DMPC lipid bilayer coating remains stable on a silicon substrate at 21 °C in its ordered state (L_{β} , P_{β}) with a d-spacing of 66 Å, but detaches almost completely from the solid support at 38 °C in its chain-disordered state (L_{α}). By contrast, oligolamellar lipid bilayers remain stable on a substrate at 38

°C when incubated with a solution of HA in D₂O. Lamella transformations occur over time, resulting in a new lamella phase with a d-spacing of 233 Å. This effect has to our knowledge not been reported before on solid-supported oligolamellar systems. We will discuss potential consequences of the "new" lamella phase with respect to further insight into joint lubrication.

5:20pm NT+AS-WeA11 Neutron Reflectometry, QCM-D, and TIRF Study of the Interaction of Endoglucanases with Films of Amorphous Cellulose, *M. Kent*, Sandia National Laboratories **INVITED**

Cellulase enzyme cocktails include exoglucanases that digest cellulose chain ends and endoglucanases that cleave randomly at interior points along the chains. While it is known that these enzymes work synergistically, the details are not fully understood. In addition, cellulose binding domains (CBDs) are known to play an important role in the digestion of crystalline cellulose but much less is known about the benefit of CBDs in the digestion of amorphous cellulose. Amorphous cellulose is of interest as pretreatment of biomass with ionic liquids, a promising next generation technology, results in a combination of amorphous cellulose and cellulose II. Determining the full effects of endoglucanase activity is challenging because these enzymes can alter the structure of insoluble cellulose in addition to releasing soluble oligomers. To unravel the actions of endoglucanases and the role of cellulose binding domains in enhancing activity on amorphous cellulose, we have combined studies of the profile of water through cellulose films during digestion by neutron reflectivity, measurements of changes in mass and film stiffness using a quartz crystal microbalance (QCM), and visualization of the motion of individual enzymes by total internal reflection fluorescence (TIRF) microscopy.

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