Solid State Molecular Science

Professor John White

Neutron and X-ray scattering methods developed by this research group are used to study the structure and dynamics on the nanometre and picosecond space/time scales. Adsorption, self-assembly at interfaces, polymers, the imitation of biomineralisation phenomena using "template" molecules and, most recently, the structure and denaturation of proteins at interfaces are current areas of interest. The insights gained are used to guide chemical synthesis in making new materials with interesting physicochemical properties. One recent highlight has been the first determination of the thermodynamic parameters for protein denaturation in the 50 Angstroms surface layer of a protein solution. By comparison with denaturation in the bulk, the contribution of the surface forces can be measured quantitatively. Another is the first measurement of the interfacial structure of an emulsion surface by neutron reflectivity. "Micro breaking" of the emulsion at the interface with a solid surface has been detected.

Our collaboration with Orica Ltd and Food Science (Australia) on the structure and stability of emulsions has produced scientifically interesting and practically useful information. We continue to show that structural relationships at the nanoscale have importance for rheological and other properties.

The Growth of Highly Ordered Titania- and Zirconia-based Films at the Air-Water Interface

Growth of highly ordered silicate films at the air-water interface have led to the development of new metal oxide films based on titania and zirconia. The surfactant-assisted assembly of these materials at the air/water interface has been monitored by fast time-resolved X-ray reflectometry using an instrument in an energy dispersive arrangement, constructed recently at the Research School of Chemistry. The new films were robust enough to be characterised by scanning electron microscopy, energy dispersive spectroscopy and small angle scattering using X-rays and neutrons. *(with M.J. Henderson, D. King, A. Rennie [NFL, Uppsala Universitet Sweden], and N. Rosier [Universite Paris-Sud])*

The Energy Dispersive X-ray Reflectometer

This instrument is now configured to obtain a **Q**-range of 0.05 - 0.4 $Å^{-1}$ with a **Q**-resolution approximately 2%. This has been achieved with the use of a liquid nitrogen cooled Li-Ge diode detector in place of the Bragg rotor. With X-rays incident onto the sample at ca. 0.6°, this arrangement permits time-dependent behaviour to minute resolution from either strong Bragg diffraction from the metal oxide films or from the broad fringes characteristic of surface excess of protein monolayers at the air/water interface to be monitored. *(with M.J. Henderson, D. King and A.W. Perriman)*

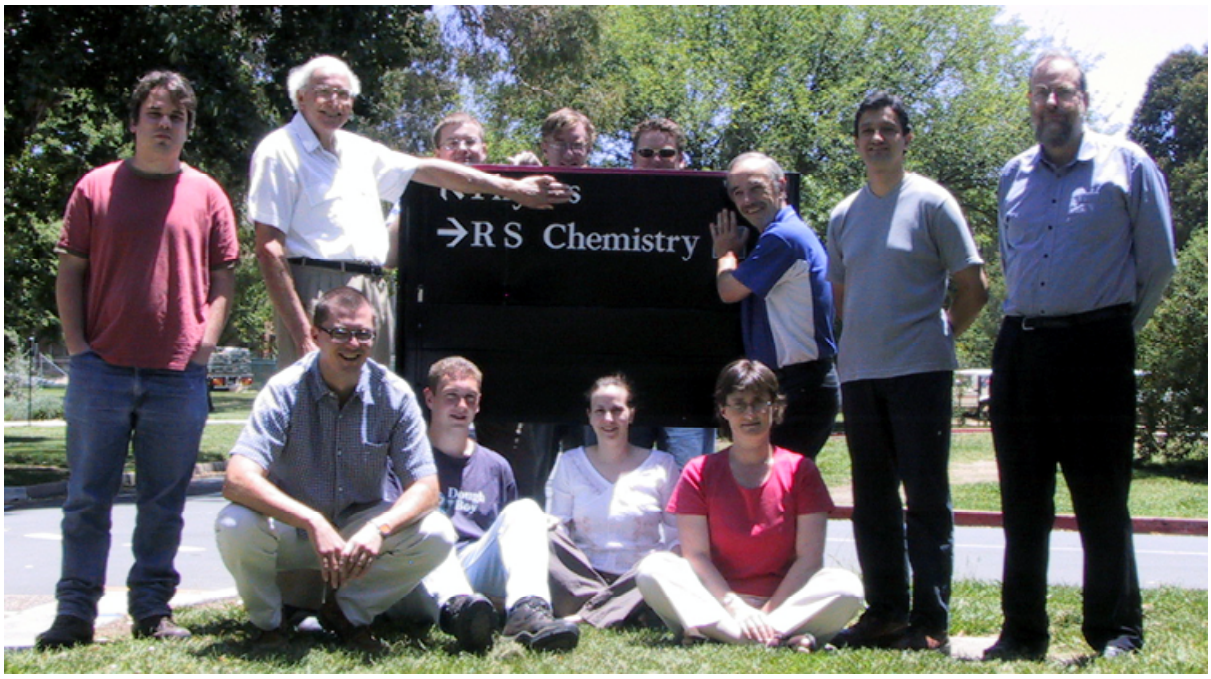
Solvent Effects in High Internal Phase Emulsions

Our previous work using small angle neutron scattering (SANS) and neutron and X-ray reflectometry on high internal phase emulsions has shown that these consist of polydisperse micron-scale aqueous droplets, 90% by volume, suspended in a continuous 10% by volume hexadecane oil phase. The polyisobutylene based surfactant stabilizes

the droplets within the emulsion by monolayer formation at the aqueous/oil interface, and by formation of nanometer-scale reverse micelles within the oil phase. We have begun investigation of variation in the oil phase by collection of complete sets of SANS data within the phase space hexadecane-toluene-cyclohexane as a function of temperature, both from emulsions and microemulsions. Even at this early stage of analysis strong solvency effects are obvious. Some oil contents promote emulsion instability or suppress emulsion formation. *(with K. Baranyai, M.J. Henderson, J. Zank, P.A. Reynolds, and A. Lafontaine [Universite Paris-Sud])*

Ultra Small Angle Scattering from High Internal Phase Emulsions

SANS probes scales from ca. 1 to 50 nm in high internal phase emulsions, while optical methods probe scales greater than ca. 1000 nm. Structures on scales of 50 to 1000 nanometres are, for technical reasons, not visible by use of electron microscopy, but are potentially so by the use of Ultra Small Angle Neutron Scattering (USANS). Coverage of this gap between SANS and optical microscopy potentially provides a complete structural description. Apart from unexpected structures, we already believe that in this gap there are small aqueous droplets, of unknown minimum size and surfactant aggregations. We have used the USANS instrument BT-5 at NIST to provide preliminary data from 20000 nm down to 60 nm on high internal phase emulsions with various neutron contrasts. *(with M.J. Henderson, J. Zank and P.A. Reynolds, and J. Barker [NIST])*



Standing from left to right: Krisztian Baranyai, John White, Andrew Jackson, David King, Adam Perriman, Gordon Lockhart, Mark Henderson and Philip Reynolds. Seated from left to right: Hans Zank, Adrian Hawley, Nikki Johnson and Val Wayte

http://rsc.anu.edu.au/research/white.php