"A Feast of Polymer Physics"

University of Leeds, Leeds, U.K.
January 17, 2007

In celebration of the lifetime achievements of three distinguished physicists from the Polymer IRC, a one day symposium was held at the University of Leeds in January. An international collection of speakers, many of whom collaborated with Geoff Davies, Alan Duckett and Mike Brereton over the years, was brought together to share their own latest research and their memories of working with them. Over their careers, Professor Geoff Davies, Dr Alan Duckett and Dr Mike Brereton have contributed enormously to the success of the Polymers and Complex Fluids Group in the School of Physics and Astronomy at the University of Leeds and all are original members of the internationally renowned Polymer IRC.

■ **Professor Geoff Davies**' research interests included electrostrictive elastomers, polymer gel electrolytes, hyperbranched polymers, the simulation of relaxations in glassy polymers and semi-crystalline polymers. Geoff was one of the founding members of the Polymer IRC and was Associate Director at Leeds for eight years.

■ **Dr Alan Duckett's** research has been concerned with the structure and property relationships for polymers and polymer composites and gas diffusion through polymer films. In his work with the Polymer IRC Alan has worked closely with chemists at Durham and engineers at Bradford and many industrial partners for over thirty years.

■ **Dr Mike Brereton** has spent many years investigating NMR properties of polymer molecules as a theoretician. His work has involved long-term collaborations with groups in Halle and the Max Plank Institute for Polymer Physics in Mainz, where he has spent the summer months for more than 10 years. He has also contributed greatly to the theory of entanglements in polymeric fluids.

Professor Ward congratulates Alan Duckett, Geoff Davies and Mike Brereton.

After a reflective introduction by the Director of the IRC, Tom McLeish, who delved into his own personal experiences of working with the three retirees, Geoff gave an overview on one of the last areas of research before his retirement, the modelling of relaxations in glassy polymers, in particular the identification of the possible molecular motions which lead to sub-Tg transitions in such polymers as polypropylene. This was followed later by his last student, Jean-Claude Berthet, who further elucidated this work using a quasi-static technique applied to methyl and methoxy rotation in PVME.

Greg Rutledge from MIT rounded off our morning session with a talk entitled "Polymer Crystallization from a Molecular Perspective" in which he outlined a non-equilibrium molecular dynamics simulation algorithm to model crystal growth in long alkane chains. He demonstrated how this approach can be used to extract crystal growth rates as a function of both temperature and molecular weight. In addition, he introduced a generalisation to flow induced crystallisation, which models the effect of chain deformation on both nucleation and growth. Professor Greg Mckenna gave an enthusiastic discourse into an apparent violation of the third law of thermodynamics. The Kauzmann paradox describes the condition in glass-forming polymer liquids where the entropy of these systems appears to collapse too rapidly as Tg is approached, with the result that the entropy can become less than the entropy of the crystal; the temperature at which the excess entropy goes to zero gives the Kauzmann temperature TK. By performing absolute measurements of the heat capacity of mixtures of poly(·-methyl styrene) and its oligomers, the

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changing entropy as a function of concentration and temperature could be ascertained. It was found that there is no "ideal" glass-like transition in entropy at temperatures far below the Kauzmann temperature, implying that TK may not be explicitly linked to the glass transition event itself.

After this surge of theory and experiment, Alan Duckett smoothed the pace of the proceedings with some absorbing reminiscences of his time at Bristol University under the tutelage of Cecil Frank Powell, who was awarded the Nobel Prize for Physics for his discovery of the pi-meson. The lunchtime plenary was led by Professor Ian Ward, who offered some of his own experiences of working with Alan, Geoff and Mike.

Beginning the afternoon session, Alessio de Francesco, a former student of Alan's, described a new neutron spectrometer built from scratch at ILL named BRISP. Principally this device makes use of Brillouin scattering for biological systems with a view to measuring changes in dynamic structure factor induced by temperature, pressure and magnetic field. Mike Brereton spoke on the research problems that remained unresolved as retirement approached. One area on which he deliberated was in determining an exact analytical evaluation of the multiple quantum NMR sine-sine relaxation function which in consequence appears to offer the extraordinary possibility of compressing a polymer dynamic time scale of three to four orders of magnitude into a single (one order of magnitude) NMR experiment.

To end the proceedings, a latest examination of the phononic properties of colloidal crystals was given by Professor George Fytas from the Max Planck Institute. These self-assembly systems reveal, via Brillouin light scattering, two phononic band gaps when thermally excited by acoustic waves and simultaneously exhibit phononic and photonic band gaps in the visible spectral region. This exceptional material characteristic has implications for future technological applications such as acoustic-optical devices.

One of the most significant advances in terms of polymer rheology, which lies at the heart of research in the Polymer IRC, has been the synthesis of model materials in such sufficient amounts that a range of analytical techniques can be then brought to bear. The model polymers developed so far have ranged from monodisperse, linear or topologically more complex structures such as combs and stars, branched materials, dendrimers, and blends thereof, with specified chain and branch lengths. Indeed, the ultimate objective, that of securely modelling the dynamic flow of molten polymers in various realms of shear and extension has been assisted inordinately by the preparation of polymer topologies and blends which are predicted to give particularly interesting dynamics under flow. Another aspect is the scaling down of analytical devices where quantity of material is an issue; the Multipass Rheometer has enabled stress birefringence, SANS, velocimetry and particle tracking on small amounts of speciality polymers in extensional flow using a range of geometries. Lately, extensional fixtures which can be integrated into a standard melt rheometer have allowed superficial access to high elongational rates. This has implications for matching industrial processes and for modelling the flow regimes therein; a clear challenge for polymer scientists, engineers and mathematicians is to bridge the gap between these "micro" and "macro" environments, something to which the Polymer IRC has formally dedicated itself.

The archive and gallery of the "Feast of Physics" can be explored further on: http://www.irc.leeds.ac.uk/feast/feast.htm

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