

(Florida State), described a brief history of the development of the Tobacco Mosaic Virus structure which included cryoelectron microscopy, 3D image reconstruction and fibre diffraction using SR. Pierre Rizkallah (Daresbury) described his current work on the tetrameric/dimeric structure of Lectins and their importance in HIV research as anti-viral agents. Peter Williams (Kings College) gave the final talk by describing his work on the structure of PLB which has been identified as a convoluted bilayer in the form of a tetrapod, joined together as a diamond cubic lattice.

John Squire concluded the meeting by awarding the

prizes for the best poster presentations (as judged by D.Caspar, S.Rastogi and B.Hsiao) to Patrick Fairclough (UMIST) and Liam Welsh (Cambridge). A special vote of thanks was made to Val Matthews and Diane Travis for all the hard work and organisation that went into making the whole meeting run smoothly.

A fuller account of the talks/posters presented at this workshop may be read later in this volume or viewed on the World Wide Web at:

<http://www.dl.ac.uk/SRS/CCP13/workshop97>.

Geoff Mant

## **Third Fibre Diffraction Workshop Kentucky, USA, 5-8 October 1997**

A group of fibre diffractionists gathered at Jenny Wiley State Park, Kentucky, USA, during 5-8 October 1997, for the "Third Fiber Diffraction Workshop." This was the third in a series of highly successful workshops, the first being held in Tennessee in 1989 and the second in Indiana in 1993. The emphasis of the workshops has been on methodology, since this is often not emphasised at other crystallographic and specialist meetings. In addition to the U.S. participants, there was a rather large turnout from the U.K., as well as one participant (Consiglia Tedesco) from Italy. The workshop was sponsored, as were the previous ones, by the du Pont Company.

Highlights of the workshop were descriptions of the uses of neutrons to study water structure around DNA (Trevor Forsyth) and bacteriophage structure (Magdalena Ivanova), and X-ray synchrotron radiation for microfocus and time-resolved studies (Watson Fuller and A. Mahendrasingam); as well as a description of the instrumentation and facilities for fibre diffraction at the SRS (Elizabeth Towns-Andrews). Gerald Stubbs used examples from virus structures determined by fibre diffraction to address the question: What are the limits of fibre diffraction analysis? He concluded that recent successes have not yet defined the limits of molecular replacement approaches in fibre diffraction, and that continued vigilance is needed in assessing the accuracy of structural results.

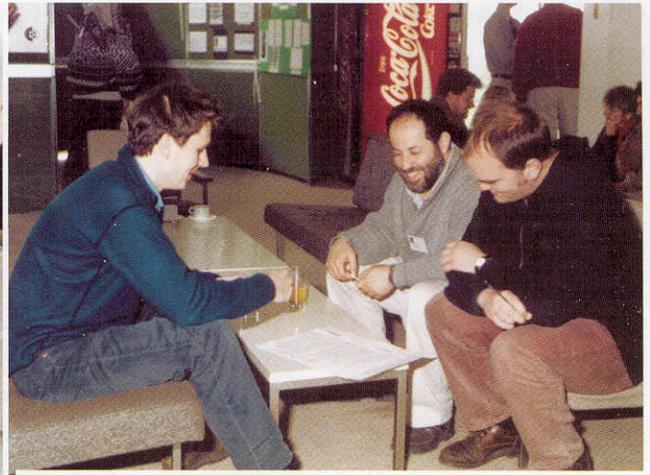
Hong Wang and Richard Denny updated us on software systems for processing fibre diffraction data. The various kinds and degrees of disorder present in fibre specimens, ways of modelling them, and their effects on diffraction data and structure determination were discussed by Rick Millane and Jon Eads.

The structures of a variety of synthetic polymers were described, including fluoropolymers (Soo-Young Park), polyamides (Kenn Gardner), and copolyester-amides (JaeDong Cho), as well as studies of variations in orientation and crystallinity of PET and LDPE both across container walls and during drawing.

The wide applicability of fibre diffraction techniques was illustrated by descriptions of various aspects of applications to viruses, bacteriophages, nucleic acids (Akella Radha), actin (Rebecca Page), amyloid (Mark Bartlam), polysaccharides (Victoria Finkenstadt), deoxy-hemoglobin (Xiang-Qi Mu), liquid crystals (George Mehl), and various synthetic polymer structures.

The meeting concluded with unanimous agreement to hold a fourth workshop, probably in the year 2000.

Rick Millane



## Photographs

*Bob Pendlebury describes a new ICI polymer fishing line suitable for mendacious anglers. Don Casper peruses this year's posters, while Norbert Stribeck reminisces with Greg Diakun about the SAS96 meeting in Campinas. Patrick Fairclough receives his prize, confirming the Ryan group domination of the polymer poster competition.*

## Perfect Plastic Products Need Good Crystal Management Proceedings of Royal Society 1997

It is all too easy to take for granted something as simple as plastic sachets used in coffee and tea machines. In reality, it can take some complex polymer science to get the right material properties for the sachets and, just as important, to maintain those properties from batch to batch. Polymer processors now have a better understanding of how they can achieve these goals thanks to a research project carried out by the Manchester Materials Science Centre at UMIST and the Daresbury Laboratory of the Council for the Central Laboratories of the Research Councils (CCLRC).

The ROPA project was on show at this summer's prestigious annual summer exhibition at the Royal Society. The exhibit was a 2/3 scale model of the experiment on beamline 16.1 at the SRS. To make the exhibit work visually the data was played back from video on screens placed in the detector housing. There were many other interesting exhibits at the exhibition but there was little time to enjoy them as the days were spent explaining the research to members of the public (mainly OAPs and schoolchildren) and the evenings dedicated to Fellows and their guests.

The UMIST team, Nick Terrill, Patrick Fairclough, Bob Young and Tony Ryan, in collaboration with Liz Towns and Ernie Komanschek of CLRC investigated the way in which polypropylene crystallises during extrusion to produce polymer films using 2D SAXS/WAXS during extrusion. Analysing the scattered radiation allowed the UMIST group to create what were in effect movies of what was happening inside polymers as films formed through extrusion.

Crystal growth itself is well understood. Indeed, as Tony Ryan points out, it is a part of undergraduate

teaching. Nucleation is another matter. "Understanding of the nucleation step is far from satisfactory" says Ryan, who has just moved to Sheffield University along with Fairclough and Terrill. So they decided to study this in a ROPA project.

The team made both small and wide angle scattering measurements on polypropylene and other polymers. The researchers built an extruder that let them study the polymer in conditions like those produced during commercial processing. Wide angle X-ray scattering (WAXS) allows researchers to study the development of structure at the atomic level while small angle X-ray scattering (SAXS) is suitable for studying the larger length scales associated with orientation of the polymer crystals. CCP13 software is used to extract the information from the noisy data. One surprise finding of the work on the SRS was that there were signs of long range order developing before crystallisation began and created short range order. There are two papers in press, one dealing with the experimental observations and the other outlining a phenomenological density of states theory for spinodally assisted crystallisation. These papers should provoke some controversy and energise the academic field of polymer crystallisation for some time.

The research has not only added to the understanding of the process of polymer crystallisation, it has already produced commercial benefits. A company making sachets for coffee vending machines has improved its products thanks to the better understanding of polymer processing. As a result of the UMIST work, the sachets now break and deliver the contents in a more controlled way.

Tony Ryan