Editorial Policy

Articles for inclusion in the Fibre Diffraction Review are welcome by the Editor at any time, but preferably items for the December 1997 issue should arrive before the end of November 1997. It is hoped that the Fibre Diffraction Review will become an Annual 'essential' for Fibre Diffractionists. This is the place to advertise your fibre diffraction or NCD meetings, to report on new software or 'hot' results obtained using the CCP13 or other fibre pattern processing suites and to provide reports of meetings of interest, preferably together with one or two photographs. All technical articles will be scrutinised both for scientific content and presentational style by the Editor (or his nominee) together with at least one other member of the CCP13 Steering Panel. In this way we hope to maintain high standards. Remember that the Newsletter not only goes to other Fibre Diffractionists, but also to various members of the Research Council Secretariats and to other funding agencies.

International Cooperation

Although these CCPs are UK funded projects, there is a very strong interest in making them international through cooperation with interested scientists in other countries. A natural link for CCP13, for example, exists with the Special Interest Group (SIG) in Fibre Diffraction of the American Crystallographic Association and possibly with some American synchrotron users (CHESS). Others exist with the ESRF at Grenoble and with the Photon Factory in Japan.

Retirements and New Elections

At the 1996 Annual Meeting, John Squire was re-elected as CCP13 Chairman, Geoff Mant was re-elected as Secretary and Manolis Pantos was re-elected as a Committee member. Unfortunately, Dr. Rob Rule tendered his resignation from the Committee in November 1996. Rob's job has moved and he now has new commitments that make it difficult for him to continue. However, he has made a major contribution to our activities for a number of years and I am happy to express, on behalf of CCP13, our considerable appreciation of his role in helping to get CCP13 off the ground and into the healthy position that it now enjoys. The CCP13 Committee are now seeking a replacement for him. The term of office of Tony Ryan finishes at the May meeting this year; other existing Committee members all continue at least until 1998. There are therefore two positions to be filled at the CCP13 Annual General Meeting in May. Tony Ryan is prepared to stand again for election to the Committee. Other nominations for election to the Committee can be sent to the CCP13 Secretary, Dr. Geoff Mant, before the May 1997 meeting.

John Squire

IF YOU ARE A FIBRE DIFFRACTIONIST STUDYING SYNTHETIC OR BIOLOGICAL POLYMERS. THIS CCP IS FOR YOU. PLEASE HELP TO MAKE IT WORK!

1996 IUCr, Seattle

The main focus of this CCP13 sponsored visit over 10 days (August 12-22, 1996) to the USA was the attendance and presentation of an invited paper at the XVII IUCr (International Union of Crystallography) meeting in Seattle, Washington. This esteemed crystallography conference which boasted the participation of no less than eight Nobel Prize winners took place in the magnificent Washington Convention Centre over a period of nine days, the last four of which were attended. Arriving on the "rest day" I dutifully relinquished the Panoramic Tour of Seattle to give a seminar at the Centre of Bioengineering (University of Washington) where I was most warmly hosted by Gerry Pollack. The fibre diffraction session comprised three sub-sessions including 27 papers covering synthetic polymers (chaired by Kenn Gardner), methods of structure determination (chaired by John Blackwell) and fibre diffraction of biological polymers (chaired by Rick Millane). Reports and abstracts from these sessions are all available on the IUCr WWW page (http://www.hwi.buffalo.edu./aca/).

In the final session on biological structures K.Namba discussed the complimentary use of X-ray fibre diffraction and electron cryomicroscopy to deduce the domain structure of the flagellin subunit in the flagellar filament; this revealed an overall folding of flagellin and direct interaction of the termini in the very inner core of the filament. M.M.Tirion discussed the use of two different methods in the refinement of the F-actin structure against 7Å X-ray fibre diffraction data. Both methods showed similar trends in the structural changes of G-actin to F-actin, including the closure of the nucleotide pocket between the large and small domains. M.Ivanova had a busier afternoon than most, presenting two talks; firstly on X-ray and neutron diffraction studies of filamentous bacteriophage M13 and Pf1 and chemically and genetically constructed variants of these particles, a topic which was widely covered with an additional contribution from G.Stubbs on his recent studies of site-directed mutagenesis of tobacco mosaic and other filamentous viruses, and secondly on a method of background estimation of these data. This uses the observation that the spatial frequencies making up the background are much lower than those that constitute the data. Iterative low pass filtering to separate the layer line data from the background and integration of this process into angular deconvolution allowed accurate estimates from patterns that could not be successfully processed by previous methods. K.Okuyama described the structural analysis of hydrated chitosan derived by deacetylation of chitin tendon showing that the transition from the hydrous to the anhydrous form requires cleavage of the NH-O6 hydrogen bond between antiparallel molecular chains and the formation of the new NH-O6 bond between parallel polymer chains. L.C.Yu showed that detailed analysis of the inner region of the first layer line in X-ray patterns from fibre bundles of skinned rabbit psoas suggests that the layer line is a mixture of overlapping thick and thin filament based layer lines and their relative contribution varies with ionic strength, correlating with the fraction of weakly bound cross-bridges. The diffuse scattering is little effected by these changes supporting the idea that the weakly attached cross-bridges assume nonstereospecific conformations. There were many other papers of particular interest on muscle and membrane protein structure and the techniques used in their crystallisation and determination. In the session on *Muscle & Motor Proteins,* C. Smith presented the recently published structure of a fragment of myosin cross bridge crystallised with ADP vanadate as an analog of the transition state complex; this being the expected form of the cross bridge at the beginning of the power stroke. Possible conformational changes following the release of ADP during the power stroke are suggested by the high resolution cryo-electron microscopy of actin decorated with myosin cross bridges. R.Milligan showed that on addition of ADP to this preparation the distal lever arm of the cross bridge rotates through 35°.

A final very full day in Seattle at the loftiest heights of the Olympic Peninsula was followed by the presentation of a paper at the Whistler Centre for Carbohydrate Research at Purdue University (West Lafayette) where I was very kindly hosted by Rick Millane. Grant Bunker (director of BioCAT, Biophysics Collaborative Access Team) very kindly hosted a visit to the Advanced Photon Source (APS) at the Argonne National Laboratory. The BioCAT beamline, under construction at the time of this visit, will provide X-ray diffraction/scattering and X-ray absorption spectroscopy for studying biological structures and dynamics at the molecular level. Its main focus is non-crystalline systems, with an emphasis on time-resolved experiments and studies of small ordered domains (down to 50-100μm). The beamline will deliver 2.4×10^{12} ph/s/mm^2 without focusing of the incident beam and 5×10^{14} with the beam focused at the specimen position with a spot size <50μm (FWHM vertical) by <200μm (FWHM horizontal). The director, Grant Bunker, has assembled a very talented team including Tom Irving, Edgar Black who was in charge of engineering and installing most of the magnets in the ring and Gerd Rosenbaum who built one of the first synchrotron X-ray beamlines about 25 years ago at DESY in Hamburg for fibre diffraction studies of muscle. The remaining two days were spent on an excursion through Toronto and finally a seminar presentation at the Materials Science and Engineering Dept. of Lehigh University in Bethlehem (Pennsylvania). The next IUCr conference in 1999 will be held in Glasgow organised by Chris Gilmore.

Jeffrey Harford