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## THE 1st WORKSHOP - BIRTH OF A NEW CCP

### *CCP13 in FIBRE DIFFRACTION*

The first of what is planned to be an annual series of CCP13 Workshops on Fibre Diffraction was held at the Daresbury Laboratory on 15 and 16 May 1992. There were over 40 registered participants.

#### FRIDAY MAY 15th

In his introduction, the Chairman explained the purpose of CCP13 as follows:-

- To develop a suite of fibre diffraction programs for general circulation and implementation by CCP13 members.
- To inform CCP13 members of software developments in their area.
- To organise workshops on fibre diffraction (with a strong emphasis on teaching).
- To promote interaction and collaboration between UK fibre diffraction groups and to establish links with interested groups overseas (e.g. with ESRF, DESY, the fibre diffraction special interest group (SIG) of the ACA, the Photon Factory).

There followed two talks on the current status and future plans for fibre diffraction work at Daresbury (Joan Bordas) and at the ESRF (Christian Riekel), after which there was a session on high resolution fibre structures. Don Marvin (Cambridge) talked about recent results from filamentous bacteriophage, Ken Holmes (MPI, Heidelberg) talked about the actin filament structure and Watson Fuller (Keele) presented time-resolved diffraction work on DNA and on the polymer PEEK. Talks on methods during this session were given by Paul Langan (Keele) on the application of Patterson methods in DNA studies, Michael Lorenz (Heidelberg) on the new software package PROFIDA that was used to analyse with Ken Holmes the diffraction patterns from actin gels and Alex Stewart (Brandeis) on a possible file structure for the new 'FIBRE' suite of programs.

On the evening of the 15th, drinks and conversation were enjoyed in the evening sunshine overlooking the canal and looking towards western Cheshire. This was followed by an excellent dinner and a spectacular sunset!

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## SATURDAY MAY 16th

The Saturday session started with a series of talks on the current status of various area detectors of use to fibre diffractionists (apart from film!). Rob Lewis (Daresbury) spoke about the rapid progress being made with multiwire proportional counters, Chris Hall (Daresbury) discussed his comparisons of various commercial image plate systems, and Simon Hanna (Cambridge) described his application of CCD detectors to 'diffractometry' of oriented polymer specimens. The session was completed by a quick resume by Wojcieck Wolf (Daresbury) of how CCP4 in Protein Crystallography operates and what the CCP4 programs are.

After coffee there were a number of talks on low-angle fibre diffraction studies; Tim Wess (Edinburgh) spoke on collagen fibril structure, Jeff Harford (Imperial College) discussed recent time-resolved diffraction results from fish muscle and new methods for analysing the observed data and John Harries (Daresbury) presented work on frog muscle, including impressive new data from 'image plate' experiments. The session concluded with two talks on software. Geoff Mant (Daresbury) talked about the new BSL package, implemented for UNIX workstations, and Alex Stewart (Brandeis) discussed some new approaches to analysing muscle diffraction patterns.

After lunch there was a general discussion on how CCP13 should proceed. The Chairman reported that the CCP13 Steering Panel (see below) had set up a Working Group (Geoff Mant, Trevor Forsyth, Jeff Harford and Richard Denny [the CCP13 'RA']) to define as a matter of urgency a standard file format for FIBRE software. At the same time existing fibre diffraction software from different sources will be scrutinised and adapted, where appropriate, to form the core of the FIBRE suite. The first planned development of new software will be to write a program to fit asymmetric (i.e. non-circular) 2-D background scattering in fibre patterns for subtraction from 'useful' diffraction (sampled peaks, layer-lines, etc). At a later stage the modelled diffraction pattern would be refined together with a background to give an optimised fit.

At the end, the Chairman thanked Geoff Mant and the Daresbury office for all of their hard work in organising what was a very enjoyable and successful meeting. He also thanked Professor Joan Bordas for his support and all the speakers and session chairmen for their contributions.

### **ARE YOU INTERESTED?**

CCP13 is open to anyone who is interested. If you want to join us to promote fibre diffraction and to help in your own data analysis then contact the secretary, Dr. Geoff Mant, at the SERC Daresbury Laboratory, Warrington WA4 4AD, Cheshire, U.K. [tel: 0925 603169], giving your name, address, telephone number and e-mail address. You will then receive all CCP13 information including the Newsletter.