
CHAIRMAN'S MESSAGE

The current, third, edition of the annual CCP13 NEWSLETTER is bigger and meatier than ever, reflecting the undoubted success of CCP13. The articles in the Newsletter detail the progress in developing fibre diffraction software in the past year, some ideas about the direction that CCP13 should take in the future, and application of the existing suite to a range of interesting biological and materials science problems. As detailed in the article by Geoff Mant, the 1994 Annual Workshop at Daresbury was a joint meeting of CCP13 and the Non-Crystalline Diffraction community at Daresbury, reflecting the considerable overlap of interests of the two groups. The meeting was very well attended and emphasises the importance of the topic. This year we hope for an even larger audience. Remember that your poster could win a large cash prize (1st Prize - £100; 2nd Prize - £50). There will be bursaries available for students and young scientists. Details of all these are given at the end of the Newsletter.

Reminder - What is a CCP?

CCP stands for Collaborative Computational Project. CCP13 is currently funded by the UK Biotechnology and Biological Sciences Research Council (BBSRC) via its "Equipment and Facilities" office. It is one of 12 current CCPs. These are:

CCP1	Electronic structure of molecules
CCP2	Continuum states of atoms and molecules
CCP3	Computational studies of surfaces
CCP4	Protein crystallography
CCP5	Computer simulation of condensed phases
CCP6	Heavy particle dynamics
CCP7	Analysis of astronomical spectra
CCP9	Electronic structure of solids
CCP11	Biosequence and structure analysis
CCP12	Novel architecture computers in Fluid Dynamics
CCP13	Fibre diffraction
CCP14	Powder diffraction

Until recently, the general policy on CCPs and the evaluation of their progress has been considered by the CCP Steering Panel, previously chaired by Dr. Julia Goodfellow, Birkbeck College, London, UK. The Steering Panel used to comprise all of the CCP Chairpersons and various observers. However, the restructuring of the Research Councils has meant that some CCPs previously funded by SERC have now been transferred to BBSRC. This includes CCP13, together with CCP4 in protein crystallography and CCP11 on sequence analysis. Most other CCPs are now with EPSRC. Pressure is being applied by CCP chairpersons to re-establish a kind of CCP Steering Panel, but to date this has not happened.

Our current CCP runs to June, 1995. A new application was therefore made to BBSRC for continued funding. Happily this funding has been agreed and the future of CCP13 is secure until the end of September 1998. The new grant will continue the support of Richard Denny as our RA and will provide funds towards Workshops, Newsletter Production and International Interactions. Because of the considerable relevance of CCP13 to the synthetic polymer community, a separate application was submitted to the Materials Board of EPSRC. Unfortunately, although the grant was highly rated and was approved, funding for an extra 'polymer' RA was not provided. Agreed funding was towards the Workshops, Newsletter etc. Since developments on the polymer side are going to be slow without a dedicated pair of 'polymer' hands, further attempts will be made to secure funding for someone to develop 'polymer' software.

Your Contribution

Interested groups or individuals are invited to contact any of the officers of CCP13 to obtain information about CCP13 Workshops, software developments, software standards and so on. Offers of home-written software that could be incorporated into the new CCP13 suite of programs would be much appreciated and will, of course, permanently carry the authors' attribution. Make sure that you are on the CCP13 mailing list and you will be kept informed.

Newsletter Editorial Policy

Articles for inclusion in the CCP13 Newsletter are welcome by the Editor at any time, but preferably items for the December 1995 issue should arrive before the end of November 1995. It is hoped that the Newsletter 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 Suite 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.

COVER PHOTOGRAPH

A single crystal texture from orthorhombic polyethylene.

The WAXS data was taken using an image plate 10 cm from the sample with a helium filled camera. The corresponding SAXS data was also recorded on an image plate at 4.5m with an evacuated camera.

The material is a copolymer of polyvinylcyclohexane (PVCH) and polyethylene (PE). The morphology of the sample is lamella with alternating 100 angstrom layers of semi-crystalline PE and glassy PVCH. The material was oriented under shear prior to crystallisation. The confinement of the PE between glassy layers of PVCH leads to chainfolded crystals oriented parallel to the walls. The X-ray beam is parallel to the lamella and samples the PE crystals along the chain-axis. The simultaneously obtained SAXS pattern (through the hole in the image plate) confirmed the lamella orientation of the block copolymer structure and the semi-crystallinity of the PE.