

## Course Schedule

- First day    Optimization of data collection  
Morning    Instrument alignment  
              Sample preparation  
              Evaluation of experimental diffraction data  
              Instrument-induced errors  
              Sample-induced errors
- Afternoon    Introduction to the *Powder Diffraction File*  
              Alphabetic search procedures  
              Hanawalt search procedures
- Second day    Fink search procedures  
Morning    Classical powder diffraction problems  
              Phase identification
- Afternoon    Phase identification in polyphase samples  
              Solid-solution analysis  
              d-spacing calibration
- Third day    Indexing of powder data  
Morning    Quantitative analysis  
              Advanced or topical problems
- Afternoon    Computer retrieval of identifications

For further information please contact:

Ms. Josephine Felizzi  
JCPDS — International Centre for Diffraction Data  
1601 Park lane  
Swarthmore, PA 19081, U.S.A.  
(215) 328-9403

The cost of a course is \$550.00 which includes textual materials and lunches. Lodging, transportation and other costs are at the expense of the attendee.

## JCPDS — International Centre for Diffraction Data    Course Schedules

# 1988

September 20-22  
Atlanta, Georgia — Georgia Institute of Technology

November 15-17  
San Diego, California — location to be announced

## General Announcement

### The British Crystallographic Association

The BCA was created in 1982 to provide a forum for those with an interest in crystallography in all its interdisciplinary aspects, whether studied by means of X-rays, neutrons or electrons. Following the inaugural meeting at the University of Durham, the association rapidly became established, under the presidency of Professor Sir David Phillips, as the representative body of the crystallographic community

## Powder Diffraction Course

4 - 6 November 1988

SERC Daresbury Laboratory, Warrington,  
Cheshire

A short course on the collection, treatment and use of powder diffraction data for qualitative phase analysis and other applications is being offered by the JCPDS-International Centre for Diffraction Data, the Industrial Group of the BCA and the SERC Daresbury Laboratory. The purpose of the course is for the user of diffraction methods to gain proficiency in the acquisition and interpretation of experimental data and in applying the information contained in the Powder Diffraction File.

The course will emphasize the nature and organisation of the PDF and the retrieval and use of the data for characterizing crystalline materials. The importance of optimizing data collection and the implications of the accuracy of measurement of line positions and intensities will be discussed, together with the influence of instrumental and specimen induced errors. The use of both manual and computer search/match methods for phase identification will be practised through workbooks and there will be an opportunity to use the powerful CD-ROM version of the PDF for solving identification problems. The numerous applications of the PDF will mainly be illustrated by using mineralogical examples, but other classes of material, including metals/alloys, organic substances and forensic materials, can be studied, depending on the needs of the participants. The course will conclude with a session on the indexing of powder data and quantitative analysis.

The principal lecturer will be Dr. Ron Jenkins, Principal Scientist of the JCPDS-ICDD. The course will be invaluable to the novice as well as to the experienced powder diffractionist, since discussions will range from basic principles to 'state-of-the-art' techniques.

The registration fee will be £55 which includes all course materials, coffee/tea, lunches and local transport. Overnight accommodation (dinner/bed/breakfast) can be provided at a cost of £34.50 per night.

Further information and registration forms can be obtained from Dr. J.I. Langford, Department of Physics, University of Birmingham, Birmingham B15 2TT, Tel. 021-414 4662/4656.

in the UK and it is now one of the largest societies of its kind in the world.

There are four subject groups within the BCA, to cater for the diverse interests of members. These are the Chemical Crystallography Group, the Physical Crystallography Group, the Biological Structures Group and the Industrial Group. The first two operate jointly with the Royal Society of Chemistry and the Institute of Physics. The crystallography sections of these bodies formed the nucleus of the

BCA at its inception. One of the main functions of the association is to organise scientific conferences and meetings, particularly the annual Spring Meeting, at which each subject group arranges a symposium and poster session. The Spring Meeting is also the venue of a major commercial exhibition for the display of equipment, teaching aids, books and services. Other meetings, symposia, workshops, etc., mainly organised by the subject groups, enable crystallographers with similar interests to exchange information and ideas and to keep abreast of the latest developments. Members also receive a quarterly journal, "Crystallography News", which includes news, views, reports, early notices of conferences and other meetings world-wide, and advertisements for jobs and equipment.

The BCA is\* a co-operating organisation of the JCPDS-International Centre for Diffraction Data. Appropriately, the association's representative on the Joint Committee is nominated by the Chairman of the Industrial Group, since many activities of this group are paralleled by the objectives of the JCPDS-ICDD. The group was formed to bring together crystallographers from industrial laboratories and to foster liaison with university research teams. In addition to organising the industrial symposium at the Spring Conference, a meeting is arranged every Autumn at an industrial venue. The programme is biased towards industrial applications and those who would not normally present papers at scientific conferences are encouraged to contribute at this meeting. Post-graduate

students are also encouraged to attend and participate in this and other group activities, and to this end a student bursary is provided.

An important role of the BCA is the provision or sponsorship of crystallographic education, both at a popular level, through public lectures, and by means of courses for trainee or practising crystallographers. In line with the training element of the BCA's aims, the Industrial Group holds two or three 'in depth' symposia on special topics each year, where members can learn about a new technique or can acquaint themselves with an unfamiliar branch of crystallography. These highly successful symposia are run on fairly informal lines and topics covered so far include residual stress measurement, position-sensitive detectors, quantitative analysis, double-crystal rocking curves, computing in powder methods and the analysis of clay minerals. At a more basic level, an introductory workshop on identification and search/match procedures was held in 1986 and a more ambitious short course on basic powder diffraction, arranged jointly with the JCPDS-ICDD and the SERC Daresbury Laboratory, will be held in November, 1988.

J. Ian Langford  
Department of Physics  
University of Birmingham  
Birmingham, U.K.

\*or has applied to become!

## Computer Comments

*Powder Diffraction* provides this column as a service to its readers and as such, cannot be held liable for the success or failure of program software or system hardware described here. The editors reserve the right to determine the suitability of any contribution for inclusion. While this column is part of the Departments Section, it is compiled and edited by:

Roy Garvey  
Department of Chemistry  
North Dakota State University  
Fargo, ND 58105-5516, U S A  
BITNET address NU025304@NDSUVM1

to whom contributions and comments should be directed, and by:

Mark Holomany  
JCPDS-International Centre for Diffraction Data  
1601 Park Lane  
Swarthmore, PA 19081, U S A

## Our DOS Environment

When we switch on the power to our personal computer, several things happen. Lights flash and disk drives whirr into action. Our computer is executing some preliminary operations as directed by instructions stored in a Read Only Memory (ROM) containing "Basic Instructions for Operating the System". These instructions direct an initial check of the system configuration (screen, memory, keyboard, other peripherals) and initiate loading of the COMMAND interpreter, the associated Basic Input/Output System (BIOS) and the Disk Operating System (DOS) from a "system" diskette in drive A: or from "boot records" of a fixed (hard) disk drive C:. Subsequently we may be prompted by DOS to enter the "date" and "time" to initialize the internal clock. Our computing "environment" has been established and we are now ready to initiate a program to begin processing data (writing these comments, in my case).

If you are not asked (by DOS) to enter a date and time, your configuration (hardware) has been supplemented by addition of an internal clock either through original design (associated with most of the newer models) or via incorporation of a "multifunction board" (upgrading the older basic models with additional memory, data transfer ports, and other features). In the latter case, your computer may