

Correspondents Reports

Report from Czechoslovakia

Jaroslav Fiala, Correspondent

The Group for Structural Research of the Czechoslovak Scientific and Technical Society prepared a colloquium "Computational and Experimental Techniques in Structure Analysis." The colloquium, which was held in Stará Lesná, 15-19th May 1989, was attended by 124 participants, mostly from Czechoslovakia. Altogether, 61 papers were submitted, of which 28 were presented orally, at plenary sessions, and 33 at poster sessions.

The subject areas covered were crystal structure determination, chemical crystallography, structure-activity studies, statistics in crystallography, electronic-structure calculations, *ab initio* calculations of electron density distribution, proton scattering from single crystals, and, last but not least, powder diffraction.

An entire day was devoted to powder diffraction, during which the following lectures were presented:

E.K. Vasiliev (USSR): X-Ray diffraction phase analysis

J. Fiala: X-Ray powder diffractometry – historical development and present status

A. Buchal: Use of X-ray diffraction in physical metallurgy

R. Kužel: Synchrotron radiation in powder diffractometry

T. Havlík:

RIFRAN 89 – automated powder diffraction identification using ATARI 130 XE microcomputer
MIKRO Q – quantitative powder diffraction phase analysis with the use of the microcomputer ATARI 130 XE

M. Škrobán:

J. Neumann:

X-Ray diffraction monitoring of the laser surface treatment
Determination of the carbon content in steel martensite through X-ray diffraction line profile analysis

Q. Jackuliak:

J. Neumann:

Comparison of the dislocation density determination by X-ray diffraction and transmission electron microscopy

Considerable interest was aroused by the discussion of the incorrect denotation of "Bragg-Brentano para-focusing geometry" on the basis of historical documentation extended kindly by Dr. William Parrish. The chairman of the Commission on Czechoslovak Crystallographic Terminology, Dr. Š. Durovič, even proposed that this designation should be replaced by "Parrish geometry."

Short Courses and Workshops

JCPDS - International Centre for Diffraction Data

Short Course on Search/Match Methods

The JCPDS-International Centre for Diffraction Data will continue to offer three-day short courses on Search/Match methods at the Swarthmore, PA, headquarters of the International Centre and elsewhere (see attached schedule).

The courses, which are now in their 5th year, are intended to build proficiency of the user in the interpretation of experimental data, especially in the application of the information provided in the *Powder Diffraction File*. The courses should be useful to the novice as well as the experienced powder diffractionist, and all discussions start with the basic principles leading on to useful laboratory procedures. Workbooks are provided to all attendees and these contain a number of experimentally obtained X-ray diffraction data sets which are used as class exercises. During the workbook sessions, the classes are subdivided to match the needs and experience of the attendees.

The course will emphasize the nature and organization of the information in the *Powder Diffraction File* and retrieval and use of this information for interpreting experimentally collected diffraction data. The implications of the accuracy of measurement of d-spacings and intensities of experimental data with respect to use of the powder file will be discussed, as well as common instrumentation and specimen-induced errors. The use of both manual and computer search/match methods for phase identification will be practiced through the use of workbooks. Applications of File data for further characterizing phases will be illustrated using several mineralogical problems and a special X-ray diffraction minerals workbook. Other types of materials may be studied including organic and forensic materials, depending upon the needs of the participants.

Course Schedule

Day 1 Morning:	Optimization of data collection Evaluation of experimental data Instrumental induced errors Sample induced errors
Day 1 Afternoon:	Introduction to the Powder Diffraction File Role of the JCPDS-ICDD Alphabetic search procedures The Hanawalt search/match procedure
Day 2 Morning:	The Fink search/match procedure Classical powder diffraction problems Phase identification Analysis of polyphase materials
Day 2 Afternoon:	Computer techniques in data collection Use of the computer in qualitative analysis Use of CD-ROM based systems
Day 3 Morning:	<i>Continuation of problem solving session</i> Use of the Crystal data file Other data files (max-d; electron diffraction, etc)
Day 3 Afternoon:	General question and answer session

For further information please contact:

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Swarthmore, PA 19081, U.S.A. (215) 328-9403

The cost of a course is \$625.00 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

1990

February 6-8 Denver, CO – Embassy Suites Denver Airport (Hotel)

April 17-19 Florida