

Four-day National XRD Workshop

On

X-ray Powder Diffraction Analytical Methods

For

Science & Engineering Graduates

22-25 August 2009

in the

***Department of Imaging and Applied Physics
Curtin University of Technology
Bentley (Perth)
Western Australia***

Course Presenters:

***Professor Brian O'Connor and Dr Robert Hart,
Curtin Centre for Materials Research***

Overview

The course has been designed to give participants a theoretical and practical grounding in the principal characterisation methods which make use of x-ray powder diffractometry data. Approximately 60% of the course will involve hands-on instruction. Students will personally collect diffractometry data sets and then process these, both manually and with PC computers, in exercises on various analytical methods, including Rietveld analysis. While the course is relevant to the analysis of all classes of crystalline materials, attention will be devoted mainly to the analysis of minerals and ceramics.



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Western Australia

Lecture Topics and Practical Sessions

The topics to be covered in lectures and tutorials/workshops will be:

Overview (1 lecture hour)

Introduction to powder diffraction principles, practice and applications – crystallography, specimens, instrumentation, identification analysis and phase analysis. Elements of Rietveld analysis.

Principles (2 lecture hours + 2-hours practical work)

Crystallography basics, including space groups. Diffraction science, with particular reference to single crystal diffraction. Simulation of single crystal intensities – calculating structure factors. Crystal structure data bases with particular reference to the ICSD structural data base.

Instrumental (2 lecture hours + 2-hours practical work)

Specimen requirements, including preparation. The Bragg-Brentano diffractometer – optical design and alignment. Operating conditions – choice of generator settings, x-ray tube, slits, detector settings and electronics. Data reduction. Absorption (macro and micro), thick and thin samples, information depth. Preferred orientation. Extinction. Stacking faults. Use of synchrotron radiation diffraction and neutron diffraction to complement laboratory x-ray diffraction.

Identification Methods (2 lecture hours + 4-hours practical work)

Cell parameter determination and refinement; role in identification. Search/match identification analysis with the ICDD Powder Diffraction File.

Line Ratio Phase Composition Analysis (2 lecture hours + 2-hours practical work)

Traditional single-peak and multi-peak methods for thick and thin samples, including the MNI method.

Rietveld Analysis (2 lecture hours + 6-hours practical work)

Practical guide to using Rietveld analysis for crystal structure refinement, cell parameters, phase analysis, texture characterisation, strain analysis, crystallite size analysis – including mathematical basis, parameter correlations and uncertainty estimation. Rietveld phase composition analysis.

Other Diffraction Analytical Methods (2 lecture hours)

Line broadening determination of crystallite size, strain and stacking faults. Texture assessment (preferred orientation corrections). Crystallinity (amorphous content). Grazing incidence analysis. Introduction to SAXS and reflectometry.

Commercial Software Overview and Demonstration (2 hours)

Overview of software supported by instrument suppliers – PANalytical (*X'Pert HighScore Plus*) and Bruker (*DIFFRAC^{plus} Topas*).

The practical sessions will comprise exercises on –

- sample preparation
- data acquisition and processing
- search/match identification analysis (manual and computer based)
- discrete-peak phase analysis
- Rietveld analysis with the *Rietica* program

Instructors

The course will be presented by Prof Brian O'Connor and Dr. Robert Hart.

Brian O'Connor held a Personal Chair at Curtin as Professor of Applied Physics from 1990-2003 when he became an Emeritus Professor. Brian was awarded life membership of the Australian X-ray Analytical Association (AXAA) in 2000 and is the immediate past AXAA National President. He led the development of the Curtin X-ray Analytical Science Laboratory over some 30 years. Brian has an extensive publication list on aspects of x-ray diffraction analysis, including Rietveld analysis, with particular reference to minerals, ceramics and air pollutants.

Robert Hart is a Senior Research Fellow in the Centre for Materials Research at Curtin University. He has extensive experience in electron microscopy and in advanced x-ray and electron diffraction techniques. He has numerous publications in international journals in areas of inorganic synthesis and materials characterisation. He has previously worked in industry in materials processing and minerals exploration.

Course Fee and Registration

The fee for the course is \$1900, plus GST. This includes tuition costs and the provision of course materials.

Participants will be required to make their own travel and accommodation arrangements, at their own expense.

Coffee and tea will be provided during the breaks.

The number of places in the course will be limited to 16. These will be allocated on a first-come-first-served basis. Places cannot be reserved for applicants who omit to send the course fee with their registration form.

Location and Hours of Attendance

The principal venue will be the Seminar Room 301.147 in the Physics Building 301 – also designated the John de Laeter Building.

The course will be presented from 9am to 5pm each day.

Personal Computer Use

Practical classes will make extensive use of PC-compatible computers. Participants are encouraged to bring a suitable PC-type notebook/laptop machine.

Participants

The 22 - 25 August 2009 course is intended primarily for industry participants. The course will also run from 16 - 19 April 2009, primarily for Curtin University participants.- undergraduates, postgraduates and staff

While preference will be given to Curtin people for the April course and to industry people for the August course, applications will be also considered from industry for the April course and from Curtin people for the August course if there are spare places.

Enrolment Procedure

Curtin students seeking to do the course on for-credit basis are asked to enrol using the standard university procedure, and to also advise Brian O'Connor by email that they have lodged an application.

Prospective industry participants and Curtin staff and students not seeking credit for the course are asked to complete the accompanying form and return to Brian O'Connor. There is no charge for Curtin people who are using (or intend to use) the Imaging and Applied Physics XRD facilities.

Curtin University of Technology

XRD WORKSHOP
X-ray Powder Diffraction Analytical Methods
22-25 August 2009

REGISTRATION FORM

TAX INVOICE – CURTIN ABN 99 143 842 569

Please complete and return with the course fee (\$2090, including GST) to:

Professor Brian O'Connor
Materials Research Group
Department of Applied Physics
Curtin University of Technology
GPO Box U1987
PERTH WA 6845

Email: B.O'Connor@curtin.edu.au

FAX: (08) 9291 7064

Registration can be made by mail, by email or by fax.

Title: _____

Name: _____

Employer: _____

Job Position: _____

Business Address: _____

Contact Phone No.: _____

Contact Fax No.: _____

E-Mail: _____

Signature: _____ Date: _____

Registration Payment

The course registration fee must accompany the registration form. Payment by purchase order cannot be accepted

Cheque Payment Option YES/NO

The course registration fee must accompany the registration form and be in the form of a cheque made out to *Curtin University of Technology*

Credit Card Payment Option YES/NO

Credit Card Type: (Visa or Mastercard only)

Name of Credit Card Holder

Credit Card Number

Expiry Date

Please direct all enquiries to Brian O'Connor:
Telephone: (08) 9291 7067 / (08) 9266 7843
Facsimile: (08) 9291 7064
E-Mail: B.O'Connor@curtin.edu.au