PhD course:
Introduction to x-ray diffraction
with applications in materials science and metallurgy

Starts 8 September 2022 at KTH Royal Institute of Technology in Stockholm
Register here before 1 September

Purpose

This course introduces researchers in Materials Science and Engineering and related research areas to x-ray diffraction (XRD), with a focus on providing an account of the applications of XRD in materials science and metallurgy. A further aspect of the course is relating the lab-scale x-ray diffraction measurements to large-scale x-ray diffraction measurements at synchrotron facilities.

Learning objectives

After successfully completing the course, learners should have acquired:

- A fundamental understanding of x-ray diffraction (XRD) and its applications in materials science and metallurgy.
- Basic skills in lab-scale XRD preparation, operation and analysis.
- Capability to understand the scientific literature in the field to further develop, independently, their own skills in XRD characterization.
- A basic understanding of the similarities and differences between lab-scale and large-scale (synchrotron) XRD measurements.

Eligibility

The course is suitable for professional researchers and engineers with a engineering/natural science education as well as PhD students. For PhD students, the course work is equivalent to 5 credits.

Content

Lectures will cover the topics: crystallography, diffraction theory, practical aspects of x-ray diffraction measurements, qualitative phase analysis, quantitative phase analysis, microstructure analysis, applications of XRD in materials science and metallurgy, introduction to synchrotron XRD.

There will be one laboratory on practical lab-scale XRD measurements and one demonstration on synchrotron XRD measurements. Three home assignments related to the lectures, laboratory and demonstration will be handed out and should be solved by the students.

Examination

- Mandatory participation at lectures, laboratory and demonstration.
- Approved home assignments.

Literature

Primary literature:

1. X-Ray Diffraction A Practical Approach, C. Suryanarayana and M. Grant Norton.
   This book will be made available in pdf via Canvas. The book is a concise overview of x-ray powder diffraction. The lectures will also contain material from additional more elaborated literature references.
2. Hand-outs, including scientific papers and book chapters.
   The hand-outs will be made available in pdf via Canvas.

Suggested additional reading:

B.D. Cullity, Elements of X-ray Diffraction.

H.P. Klug and L.E. Alexander, X-Ray Diffraction Procedures for Polycrystalline and Amorphous Materials.

P. Staron, A. Schreyer, H. Clemens, S. Mayer, Neutrons and Synchrotron Radiation in Engineering Materials Science: From Fundamentals to Applications, 2nd Edition (this is the tentative main literature for a follow-up PhD course in Advanced XRD during 2023)

Teachers

Peter Hedström (PH), KTH, 08-790 6217, pheds@kth.se (responsible teacher)
Tao Zhou (TZ), KTH
Gabriel Spartacus (GS), KTH
Simone Sala (SS), RISE
Ulrich Lienert (UL), DESY and KTH
Fredrik Eriksson (FE), LiU

Course Fee

The course is free of charge.

Location

KTH Royal Institute of Technology. Department of Materials Science and Engineering as well as the Hultgren Laboratory.

Course registration

To apply for this course, please register here before 1 September.

Dates

Course start 8 Sept at 10 am. See schedule.

Tentative schedule September-October 2022

Time	Type	Teacher	Topic
8/9 10-12	Lecture 1	PH	Introduction to course, x-rays and XRD
8/9 13-15	Lecture 2	PH	Crystallography and diffraction theory
8/9 15-17	Lecture 3	PH	Practical aspects of lab-scale XRD measurements, including qualitative phase analysis
9/9 10-12	Lecture 4	GS	Quantitative phase analysis
9/9 13-17	Laboratory 1	TZ	XRD measurements for qualitative phase analysis
Hand in latest 21/9	Home assignment 1	TZ	Data analysis for the XRD measurements
22/9 10-12	Lecture 5	TZ	Microstructure analysis
22/9 13-15	Lecture 6	SS	Introduction to synchrotron x-ray radiation and relation to lab-scale. Overview of X-ray characterization methodologies (not only XRD).
Hand in latest 12/10	Home assignment 2	GS	Quantitative phase analysis and microstructure analysis
13/10 10-12	Lecture 7	UL?	Synchrotron XRD in materials science (instrumentation, measurements and applications)
13/10 13-15	Demonstration	GS	Synchrotron XRD data handling
14/10 9-12 TBC	Demonstration (possibly a video recording instead)	UL	Synchrotron XRD in materials science
14/10 13-15	Lecture 8	PH	Applications of XRD in metallurgy

14/10 15-17	Lecture 9	FE	Applications of XRD in thin film materials science
Hand in latest 28/10	Home assignment 3	GS	Data processing, calibration and analysis synchrotron XRD data

Acknowledgement

This course is jointly organised by the METALSF Project and the Center for X-rays in Swedish Material Science (CeXS).

CeXS is Sweden's scientific node for the PETRA III Swedish beamline located in Hamburg, Germany. CeXS partners are KTH Royal Institute of Technology and Linköping University, with Uppsala University being an affiliate from 2022. CeXS is cofinanced by the partners and financed by the Swedish Research Council.

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