PhD course: Advanced TEM Spectroscopy and Tomography

Course points: 5 HP

Course period: April-June 2018

Number of places: 10
(10 places for full course; the lectures can be attended by more participants and including collaborators from companies)

Language: English

The course purpose:
The aim of the course and its motivation is to gain a deepened knowledge about spectroscopic and tomographic techniques in the transmission electron microscope (TEM). The lecturers are experts in different fields of electron microscopy, spectroscopy, and diffraction working at the different nodes of the Center of Electron Microscopy for Materials Science, CEM4MAT, established in 2017 between KTH, SU, UU and KiMAB.

Specifically:
1) Develop skill to plan, acquire, evaluate advanced spectroscopic and tomographic experiments. 2) Understanding of basic principles of electron-matter interaction. 3) methods in TEM spectroscopy and tomography techniques. 4) Optimise the materials analysis technique to obtain best spatial, spectroscopic and temporal resolution.

The course addresses PhD students from all domains of materials science, chemistry and physics including geology. For the theoretical lectures, some background in quantum mechanics will be needed, but we try to make the course as didactical as possible.

Course Methodology:
The course will build advanced knowledge linking 8 lectures (see below for description) with 5 strong project-oriented hands-on laboratory moment. All the participants are expected to attend the lectures that will be followed by group work. Each group (2 students/group) will have a choice to work on selected materials and scientific questions that they will develop in the laboratory part. The goal is that the participants use theory part as well as recent literature to work on selected questions of materials analysis. The participants may bring their own samples to the laboratory. It is also possible to work on a theoretical laboratory project related to spectroscopy and tomography.

Course contents (2 h each lecture):

- *[TheoScat] Theoretical aspects elastic and inelastic electron scattering* (JR) This lecture will discuss the basic theoretical aspects behind scattering of fast electrons on samples. Concepts of kinematical and dynamical diffraction theory will be explained. Two-beam approximation will be used to illustrate some effects of dynamical electron diffraction. Multislice method of simulations. Inelastic scattering processes will be introduced, such as thermal diffuse scattering, plasmon scattering and core-level excitation events.

  [STEM] Scanning Transmission Electron Microscopy (CWT)
  This lecture will discuss the electron optics and image formation in scanning transmission electron microscope and their differences to the conventional one, for instant their reciprocal natures. An introduction to modern instrumentation, such as electron emitter, aberration corrector, and electron detectors will be included. In a practical aspect, the particular sample preparation and experimental procedures will be mentioned. The selected topics will help the students to have deeper understanding the methods and their potential and limitation, in order to interpret and quantify the results.

- *[EDX] Energy-dispersive X-ray spectroscopy* (FY) This lecture introduces the basic principles of energy-dispersive X-ray spectroscopy (EDX) and its current developments, followed by a discussion on spatial resolution, accuracy and sensitivity. The origin of characteristic X-rays emission as well as the properties of X-ray lines and their use in materials analysis including line identification and drawbacks compared with WDS analysis will be discussed. The detection mechanisms leading to energy resolution and detection limit in EDX spectroscopy will be explained. Limits, artefacts and possibilities to obtain chemical information down to atomic scale will also be discussed.

- *[EELS] Electron energy-loss spectroscopy, EELS* (KL) This lecture will present the background of the main aspects of EELS spectroscopy as well as their experimental realization and evaluation of spectra. The topics that will be treated in this lecture are the basic scattering geometry, the EELS spectrometer and energy filter instruments, the acquisition geometry and parameters in the TEM, typical signals in an EELS spectrum, quantification of the spectra, plasmon losses and mean free path, EELS near edge fine structure. Practical and theoretical possibilities and limits to achieve atomic resolution EELS will be discussed. We will explain acquisition conditions for EELS spectra as well as give examples from EELS spectroscopy.

- *[TheoEELS] Theoretical aspects EELS* (JR) This lecture will delve deeper into the theoretical aspects of electron energy loss spectroscopy, with particular attention to core level spectroscopy. Moller transition potentials and mixed dynamical form factor will be introduced. Dipole approximation, anisotropy of EELS and magnetic effects in EELS will be described. Methods of simulation of EELS will be briefly introduced.

- *[TomoDiff] Tomography reciprocal space* (TW) This lecture will introduce the concept of electron diffraction tomography. The lecture will cover basic concepts of the method, including data acquisition and data treatment. It will also describe theoretical aspects associated to the interpretation of the data, such as basic crystallography and the methods to be used in order to retrieve structural information from the reconstructed reciprocal lattice.

- *[TomoReal] Tomography in real space* (LX) This lecture includes: Introduction to electron tomography; conditions needed before the tilt-series acquisition on materials science samples; Tilt-series acquisition, Introduction to different methods to align the tilt-series; Tomographic reconstruction including algebraic reconstruction technique (ART), simultaneous iterative reconstruction technique (SIRT), and others; Post-processing, single particle analysis and sub-volumes averaging; Segmentation and Most recent applications of electron tomography in materials science.

- *[TREELS] Time-resolved spectroscopy* (JW) This lecture will present the concept of pump-probe spectroscopy in general and specifically applied to time resolved EELS. The topics that will be treated include photo induced near field electron microscopy (PINEM) with special emphasis on plasmonic systems. We will explain time resolved valance band and core level spectroscopy, as well as time resolved diffraction.

Labs
The labs will consist of a project work to be developed during 4-5 sessions (each session = 4 h) that will be supervised by one of the lecturers. The sessions include time at the microscope and data processing/analysis. Each project will be related to some of the lecture topics. TBC

Target group/s and recommended background
Students from engineering, material science, physics, or chemistry. Admission to the course requires knowledge equivalent to basic transmission electron microscopy course at postgraduate level, e.g. Introduction to Analytical Electron Microscopy (KZ8006 at SU) or Advanced Electron Microscopy (at UU). Recommended background quantum mechanics.

Examination
The students should write a scientific report concerning the labs, where the results are compared to the information available in the literature and theoretical aspects are

considered. The lab responsible will evaluate this report. In addition, all the groups will present their work in a conference-style seminar where all the lecturers will evaluate the presentation. The final mark will include both parts.

Responsible institutions:
- Engineering Sciences at Uppsala University (UU)
- Department of Materials and Environmental Chemistry at Stockholm University (SU)
- Applied Physics, KTH.

Lecturers:
- Klaus Leifer (KL), klaus.leifer@Angstrom.uu.se
- Jan Rusz (JR), jan.rusz@physics.uu.se
- Cheuk-Wai Tai (CWT), cheuk-wai.tai@mmk.su.se
- Jonas Weissenrieder (JW), jonas@kth.se
- Tom Willhammar (TW), tom.willhammar@mmk.su.se
- Ling Xie (LX), ling.xie@angstrom.uu.se
- Fei Ye (FY), feiy@kth.se

Contact persons and application from course participants should be sent to either
- Klaus Leifer, klaus.leifer@Angstrom.uu.se
- Germán Salazar-Alvarez, german@mmk.su.se

Deadline April 6th 2018

Schedule (date and place)

Lecture	*Lecturer*	*Date*	*Place*
[TheoScat]	JR	17/4	Uppsala
[STEM]	CWT	17/4	Uppsala
[EDX]	FY	19/4	Uppsala
[EELS]	KL	19/4	Uppsala
[TheoEELS]	JR	24/4	Stockholm
[TomoDiff]	TW	24/4	Stockholm
[TomoReal]	LX	26/4	Stockholm
[TREELS]	JW	26/4	Stockholm
Labs		To be agreed with the lab responsible	To be agreed with the lab responsible
Seminar		End of august	TBD