# IM2667 "Physics and chemistry of surfaces", 7.5 hp

## Background

Materials and their properties play a key role in todays society and technology; electronic devices and machines, catalytic reformation of chemicals, corrosion inhibition and protection, energy conversion, nanotechnology, construction materials. In many of those areas surface or interface effects are more or less important. In particular in nanotechnology it is often only the surface that is left.

### **Course content**

The course will through a selected set of examples introduce and motivate a need for a detailed physical and chemical description of surfaces on the atomic/molecular level. This includes basic surface phenomena such as adsorption, desorption, chemical bonds and chemical reactions, thin film growth and their dependence on atomic and electronic surface structure, temperature, pressure and environment.

A set of experimental surface/interface preparation and analysis methods for determination of electronic and atomic structure will be presented and described, with the aim to provide the student with a "tool-box". This box includes advanced electron and X-ray spectroscopy, electron spectroscopy, surface diffraction, synchrotron radiation and atomically resolved microscopy.

#### Lecturer and course responsible

Mats Göthelid, Materialfysik, ICT, Electrum 229 16440 Kista, tel 790 4154, gothelid@ kth.se

### Literature

"Introduction to Surfaces, interfaces and thin films", H. Lüth, Springer Verlag "Examples in Surface Science" M. Göthelid "Surface chemistry and low energy electrons" G. Ertl and J. Küppers, VCH Selected overview papers on specific topics (indicated at each lecture below)

**Exam:** home-exam. Hand-out and hand-in dates to be discussed. **Labwork:** to be discussed, when it suits your (and my) schedule

#### **Detailed contents and reading instructions:**

I will hand out paper copies from Ertl and Küppers and other literature which cannot be reached on the web, so don't spend too much time trying to find it <sup>(2)</sup>.

Lecture 1: Course information and introduction to surface science and surface analysis. What, why and how? A general overview of experimental methods and the working environment.

Read: Lüth chapter 1

**Lecture 2:** Crystal structure, surface structure, crystal bonding, surface reconstruction and relaxation. Reciprocal space in 2D.

Read: Lüth chapter 3. Revise relevant chapters from Solid State Physics if needed.

Lecture 3: Adsorption and desorption, chemical bond. Measuring the strength of the chemical bond (TPD/TDS)

Read: Lüth chapter 10

Lecture 4: Growth modes, interface structures, 2D phase transitions.

Read: Lüth chapters 3 and 10

Lecture 5: Surface Diffraction and surface atomic geometry, Scattering from surfaces, Low Energy Electron Diffraction (LEED), Surface X-Ray Diffraction (SXRD), Reflection High Energy Electron Diffraction (RHEED)

Read: Lüth chapter 4 and panel VIII

"Surface structure determination by X-ray diffraction" R. Feidenhans'l, Surface Science Reports 10 (1989) 105, http://www.sciencedirect.com/science/article/pii/0167572989900022

"Surface holography with LEED electrons", K. Heinz, U. Starke, J. Bernhardt, Progress in Surface Science 64 (2000) 163, http://www.sciencedirect.com/science/article/pii/S0079681600000113

"Surface chemistry and low energy electrons, chapter 3", G. Ertl, J. Küppers

- Lecture 6: Electron levels and electronic structure, inner levels and valence levels, band structure and surface electronic structure, surface states. Experimental techniques, angle resolved photoelectron spectroscopy and Inverse photoemission spectroscopy, Optical spectroscopy
  - *Read*: Lüth chapter 6 "Inverse photoelectron spectroscopy", G. Ertl and J. Küppers, chapter 7

- Lectures 7-9: Core level spectroscopy, elemental and chemical analysis, X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), X-ray emission spectroscopy (XES). Electron mean free path, electron analyzers and light sources. Synchrotron radiation. Structural methods based on core level spectroscopy NEXAFS, EXAFS, PED. PEEM and LEEM.
  - Read: "X-ray emission spectroscopy and density functional theory studies of adsorbates on surfaces", A. Nilsson, L.G.M. Pettersson, Surface Science Reports 55 (2004) 49 http://www.sciencedirect.com/science/article/pii/S0167572904000573

"Everything you always wanted to know, but never dared to ask about SEXAFS", J. Stöhr

Bianconi "Surface X-ray absorption spectroscopy; surface EXAFS and surface XANES" Applications of surface science 6 (1980) 392 http://www.sciencedirect.com/science/article/pii/0378596380900240

- Lecture 10: Surface microscopy: Scanning tunnelling microscopy (STM), Atomic force microscopy (AFM), Scanning electron microscopy (SEM) and transmission electron microscopy (TEM)
  - Read: Lecture 10a.pdf, Lecture 10b.pdf
- Lecture 11: Vibrational spectroscopies: High Resolution Electron Energy Loss Spectroscopy (HREELS), Infra Red Absorption Spectroscopy (IRAS), Fourier Transform Infra Red Spectroscopy (FTIR), Sum Frequency Generation (SFG), Raman Spectroscopy
  - Read: Lüth chapter 4 and panel IX

"Surface chemistry and low energy electrons" chapter 11, G. Ertl and J. Küppers,

"The dielectric theory of HREELS, a short survey", Ph. Lambin, L. Henrard, P. Thiry, C. Silien, and J.P. Vigneron, J. of Electron Spectroscopy and Related Phenomena, 129, (2003) Pages 281–292, http://www.sciencedirect.com/science/article/pii/S0368204803000793

Lecture 12: Preparation methods for surfaces and thin films.

*Read*: Lüth chapter 2