Surface Science
Nanoscience
Materials

Manual to the Power Point Class

Uwe Burghaus

Surface Science, Nanoscience, Materials
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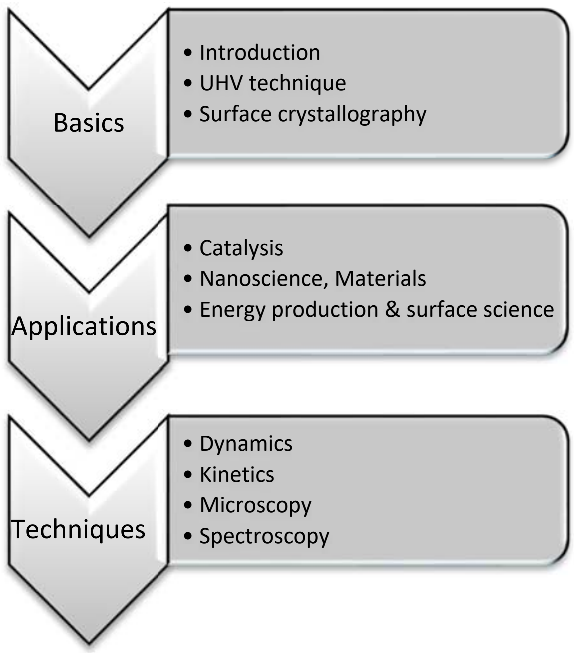
CONTENTS

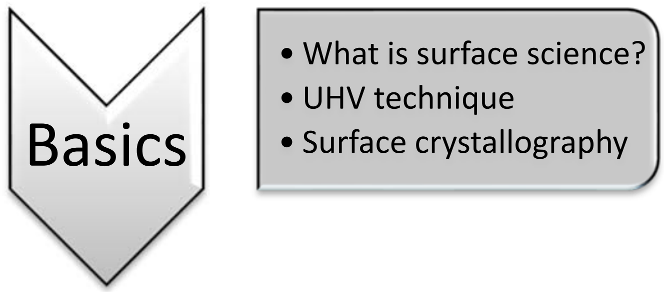
Surface Science, Nanoscience, Materials
Quick Glance
(8/15 weeks class)



Abbreviations are listed in the appendix.

CONTENTS

Surface Science, Nanoscience, Materials



A) INTRODUCTION (BASICS)________________________________

The numbering here refers to the class meetings. A meeting typically covers 2 classes (75 min)

1) Syllabus, class organization, etc.

What is surface chemistry?

Class organization is discussed 6-weeks vs. 8/15-weeks class etc. Several examples of surface science projects will be discussed ranging from kinetics and surface structure determination to dynamics. In addition, important concepts are already highlighted. Some real examples (e.g., conference talks) are provided as supplements.

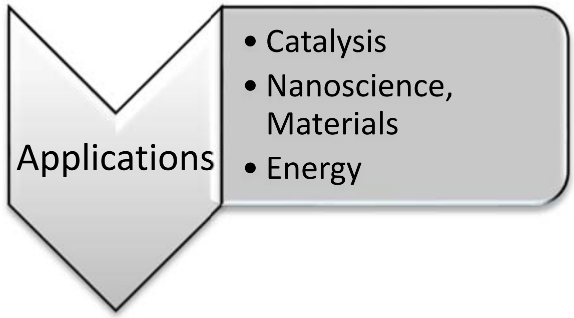
2) Ultra-high vacuum techniques

Why is a vacuum required? How are pumps working? (mechanical, ion-getter, getter, turbo, diffusion pumps), how to measure a pressure? (B&A gauge, pirani, mass specs), pitfalls (leak detection, sample holder, temperature measurements, tricks, etc.).

3) Surface/nano-crystallography

Simple structures, Miller indices, complicated structures 4-index nomenclature, crystallography of carbon nanotubes, defects, stepped surfaces, chiral surfaces, relaxations, reconstruction, Park & Maeden nomenclature, Wood nomenclature.

One could certainly add more sections here such as thermodynamics of surfaces, statistical thermodynamics, quantum mechanics of surfaces etc. I may do so over time. (Some primer of QM, thermo, solid state physics are already included.) Come back for the 2nd edition.



B) APPLICATIONS____

In particular an audience who is not exactly in the field discussed is usually interested in colorful applications rather than grey theory. I usually had a quite mixed (interdisciplinary) group of students. Therefore, I start with "applications". This approach may have some disadvantages since it is not ultimately systematic, but the advantage of keeping you engaged outranks these disadvantages, in my opinion.

4) Heterogeneous catalysis

Definition, several examples (CO oxidation, methanol synthesis, ammonia synthesis, fuel cell catalysts), the surface science approach vs. the catalysis approach, pressure/material/information gaps, experimental techniques for high pressure experiments, where is catalysis going? Outlook.

5-6) Nano-surface science (nanotechnology)

(I) Synthesis of materials

Photolithography, e-beam lithography, soft lithography, nano-imprint technique, self-assembled monolayer, nanopaticles synthesis, carbon nanotubes, inorganic nanotubes.

(II) Characterization

Electron microscopy (TEM/SEM), EDX, XRD, optical spectroscopy (absorption, IR, spectrofluorimetry, Raman), applications to carbon nanotubes, examples.

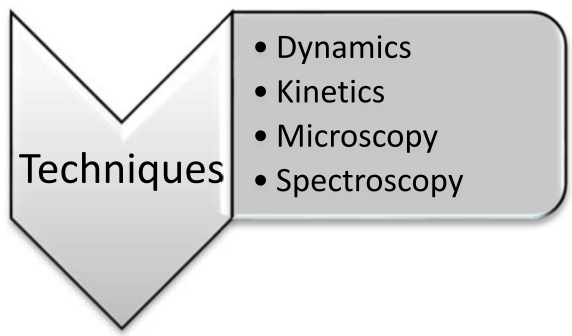
(III) Applications

Nano(heterogeneous)catalysis, model nano-array catalyst, carbon nanotubes as supports in catalysis (kinetics, dynamics, effect of crystal structure, …), simple MO theory, inorganic nanotubes (TiO_2 NT), risks (fullerenes for the face?).

7) Concepts for alternative energy production

Yes, surface science can address these problems and certainly as a modern citizen you simply have to know what is going on. Scientific background not politics will be outlined.

- **(I)** What is sustainable energy production?, global warming, CO_2 sequestration, options, solutions, fossil fuels, nuclear energy (fission vs. fusion), solar cells, semiconductors, doping, band structures, electronic structure, electron hole pairs.
- **(II)** Methanol economy, hydrogen economy, fuel cells, hydrogen production, methanol production, carbon vs. hydrogen economy, wind energy, geothermal energy, hydropower, (biofuels).
- **(III)** *Supplemental.* One example of water splitting catalysis, photo-electro-nano(?)-chemistry.



C) TRADITIONAL SURFACE SCIENCE TOPICS AND TECHNIQUES____

The rest of this surface chemistry, nanoscience, and materials class will include a discussion of traditional surface chemistry/science techniques. This may be a little boring for students who have not started to work in a research group, yet. Therefore, I started this class to outline related applications first, including nanoscience. However, if you do not learn your craft at some point, you will not make it very far in your carrier. It is essential to know most of the measuring techniques and the related theory in your field. I try to provide basic knowledge of both experimental techniques and simple methods to analyze the collected data. Note, this class was used to train new graduate students in my group.

C1. Dynamics

8) Molecular beams *(experimental)*

What is "dynamics"?, supersonic vs. effusive beam system, typical experimental set-up, energy distribution, angular distribution, advantages/disadvantages, kinetic theory of gas expansions, Maxwell-Boltzmann speed distributions, Mach number, Knudsen number, seeded beams, internal degrees of freedom, first application: adsorption probability measurements, kinetic vs. dynamic adsorption probabilities, condensation vs. adsorption coefficients.

8-9) Potential energy surface *(theory/modelling)*

(I) Basic topics

Scattering pathways: elastic, direct inelastic, trapping/desorption, adsorption; examples: He atom scattering, rainbow scattering with Ne, Ar trapping/desorption, CO trapping/desorption; basics about the potential energy surface: non-activated vs. activated adsorption, precursor mediated adsorption, 1D vs. 2D potential energy surfaces. A general-purpose introduction to PES and TST is provided as a supplemental PowerPoint.

(II) Introduction to more advanced topics

More advanced topics related to the concept of potential energy surfaces and adsorption dynamics, energy scaling laws: normal energy scaling, total energy scaling, intermediate cases; energetic vs. geometric corrugation; effect of internal degrees of freedom on the adsorption dynamics: sterical hindered adsorption, cooling of rotation/vibration degrees of freedom, vibrational mediated adsorption, rotational hindered adsorption, helicopter vs. cartwheel modes, hard sphere model, trapping mediated bond activation, state-to-state experiments.

10) Basic ideas of quasi-equilibrium and Kinetic Monte Carlo Simulations *(theory/modelling)*

Intrinsic/extrinsic precursor, precursor model (Langmuir adsorption dynamics, Kisliuk model, adsorbate assisted adsorption, cooperative effects, transient precursors), analytic models, Monte Carlo simulations, definition, averaging, boundary conditions, thermalization, energy constraint, surface defects, examples, examples, examples, time resolved Monte Carlo simulation (briefly). Software can be downloaded from my research website.

11) Time of flight techniques, molecular beam relaxation spectroscopy *(experimental)*

Using intensity modulated beams to obtain dynamics information about surface processes, TOF: basic idea, chopper function, flight time broadening, effect of surface processes, adsorption kinetics, surface reactions, examples, applications; MBRS: idea of this technique, what is a lock-in amplifier, measuring the surface residence time, reaction product vector, examples – applications (adsorption kinetics, surface reaction dynamics)

12) Surface alloys, thin films *(experimental)*

I) Motivation, terms metal-on-metal, alloy surfaces, surface alloys, adsorption, diffusion, inter-diffusion, homogeneous, heterogeneous, Frank-van der Merwe, Volmer-Weber, Stranski-Krastanov, free energy, wetting, non-wetting, equilibrium vs. kinetic constraints, less common models, Ostwald ripening, Schwöbel barrier, bulk miscible, bulk immiscible, simple trends, synergy effects, Dealloying.

II) Examples - 4 case studies

C2. Kinetics

13) Thermal desorption spectroscopy and simple related computational techniques

14) Kinetics: surface reaction kinetics studied with molecular beam scattering techniques

C3. Spatially resolved techniques / surface structure

15) Diffraction techniques

(I) low energy electron diffraction,

(II) He atom scattering (not yet included)

15) Direct techniques

(I) scanning tunneling microscopy,

(II) atomic force microscopy, etc.

C4. Spectroscopy with electrons

16) Auger electron spectroscopy

16) Photoelectron spectroscopy

16) High resolution electron energy loss spectroscopy

INTRODUCTION

In a nutshell

- Traditional surface science topics are included, but also
- Nanoscience (fabrication & characterization), and
- Materials science topics
- Another class segment is about alternative energy production and how nano/surface-science can help here
- Concepts and measuring techniques are discussed
- Focused on applications and concepts
- Chemistry, physics, engineering, material science students took this class
- Postdocs, graduate students, and undergraduates took the class
- Usually, two credit class offered in various formats (6, 8, 15 weeks)
- Power point class with extensive notes sections
- Voice recordings for most of the 6-weeks classes
- Self-study questions, homework
- Support for instructors (homework solutions, midterm, finals) on instructor CD
- ~27 PowerPoints + some supplementals
- Please note that also the PowerPoints are copyright protected. E.g., you cannot e-mail the PowerPoints to your students or a friend. If your students need a copy, they/you would need to purchase this book + CD.

Class format

Most PowerPoints for one class are an about 75 min presentation. For a full-semester two-credit class, I did usually meet only once per week, but presented a double class (50+25 min). On the CD/DVD you will find folders with the PowerPoints and homework which would correspond to a given meeting (double classes) with your class. A regular term in the US has 15 weeks (summer classes are shorter, depending on the school this may be 6- or 8-weeks classes). Thus, you may need to skip a few topics or meet a few times twice a week. Anyway, the PowerPoints include more than enough material for a two-credit class. The CD includes a 6-weeks and 15-weeks class version. If you add more interactive components, lab visits, lab sections then this can easily become a four-credit class.

Bang for your bucks (for students & instructors)

As an instructor, the PowerPoint set will save you a lot of time even if you modify the slides for your own students. Exercises, homework, and exams also are included.

As a student, the included notes sections to the PowerPoints are almost as good as voice recordings or a textbook. The shorter 6-weeks version of this class includes recent voice recordings. Thus, this class is more than just a collection of PowerPoints. This class can be used for self-study more so than a traditional textbook.

Students and instructors usually want to have a “textbook”. Therefore, I added this short “manual” to the CD/data DVD, it includes a brief summary of each class. Obviously, this is not a traditional textbook. You can find those by the dozen already, even for specialty topics such as surface science. Do students read textbooks?

Why offering this commercially?

Well, why not? I do have a part-time small business since 2013 which makes a “commercialization” rather simple. Hundreds of (private) work hours stick in this class. So, why not making it available for other colleagues, including students since I would have prepared this class anyway? In other words, the additional overhead for me for making a commercial product out of this class was moderate.

My own background

I am a physical chemist, a surface chemist, and a faculty member at North Dakota State University (NDSU), starting there in 2003. I got most of my own education in Physics in Germany, born in West-Berlin. After many years of postdoc positions (Italy, US, Italy, Germany …) and a habilitation in Germany (German tenure), I found a position at the Chemistry department at NDSU. More you can find here www.uweburghaus.us I have written several books, most of these about practical engineering topics and I sell those books in the meanwhile by myself, i.e., I do own a part time small business. Details are here www.LatheCity.com Why I market this myself? I did publish and edit books/reviews together with big and traditional publishers and probably could have found one also for this project, but simply put why should the publisher get most of the profit? The compensation publisher typically provide to authors are rather ridicules.

Conflict of interest

The PowerPoints, all texts, and this booklet were prepared in my free time.

Disclaimer

How to contact "us"

Any meaningful comment is very well-come, write to sales@LatheCity.com We will ignore harassment, nonsense, and/or spam. Also, we cannot solve your homework problems for you, sorry. ☺ Other books and original publications should be available through your university's library system we can't provide these. Our website is here: www.LatheCity.com

NOTES FOR INSTRUCTORS

Initially this class was offered solely with the purpose to train new graduate students who joint my surface chemistry group. That was in the fall semester 2005, during my second year as an assistant professor at the Chemistry Department of North Dakota State University. I had to learn rather quickly how much work it is to come up with even 15 descent PowerPoints. (A term in the US consists of roughly 15 weeks and this class was originally a so-called one credit class - one contact (/class) hour per week.) Therefore, providing these PowerPoints to other instructors and students may be appreciated. (In the meanwhile, about 30+ classes are included, and the class is offered as a 2-credit class.)

Depending on graduations and recruitment of new students, I did offer the class every few years (2005, 2008, 2010, 2015, 2021), meanwhile continuing to work on my PowerPoints. Additionally, it takes more than one run to finish that kind of class since I did not stick with a single textbook but came up with my own outline using many original works of my group and from colleagues around the world. Attracting a somewhat larger audience and acknowledging that I switched by myself in the meanwhile from traditional surface science to surface-nano/materials-science, I broadened the contents of the class including nanoscience and energy related topics (sustainable energy production). Also, the crowd became more diverse; sometimes 10 students participated from chemistry, physics, materials science, and engineering departments, including postdocs, graduate students, and undergraduates. That is pretty significant for a special topics class at a small Midwest university. (Well, in some years I have had only 4 students…) Addressing the different knowledge base, quantum mechanics, thermodynamics, kinetics, solid state physics, etc. primer were added. (However, it would be good having undergraduate level quantum mechanics as a pre-requisite for this class.) Surface science is probably among the most interdisciplinary research areas.

In the meanwhile, the class is a two-credit class (Chem472 / Chem672) and includes nanoscience, materials, and energy related topics (~30 PowerPoints). In 2010, it was offered through the distant education system of my college with additionally a dozen or so German materials science students participating. Due to copyright issues, I cannot provide these early voice recordings, but recently added voice recordings for about half of the classes. More voice recordings will be provided as these become available.

Also, I passed this class for “self-study” to visiting (summer) students or new graduate students since I cannot offer it every year. It turned out that this worked very well. The classes are stand-alone outlines: don’t remember LEED or TDS anymore? Look it up again.

For your own class, perhaps, select the PowerPoints most interesting to your research field since the class is somewhat longer than a typical term in the US.

Each PowerPoint includes (self-study) questions. Additionally, homework, midterm, final exam, etc. are also on the instructor CD. If you are an instructor, contact “us” and we send you an instructor CD with all solutions.

Acknowledgement

Some prior published results of my group related to the PhD research of Shamus Funk, Mallikharjuna Komarneni, Ashish Chakradhar, Mudivans Tilan Nayakasinghe, Nilushni Sivapragasam, and Thomas Stach at NDSU also are described on the PowerPoints as well as works of postdocs Jinhai Wang, Evgueni Kadossov and undergraduates. Their support, discussions, and work effort of the prior projects are acknowledged. Parts of the texts on the early versions of the PowerPoints were proofread by M. Komarneni.

Part of our work which also is included on the PowerPoints was originally funded by The Donors of the American Chemical Society and Petroleum Research Fund, US NSF, US DoE, EPSCoR, ND-EPSCoR, and NASA/NASA-EPSCoR. Graduate students also were supported by teaching assistantships from my university, NDSU.

The book covers were purchased from freedigitalphotos.net

List of acronyms and abbreviations – measuring techniques

AES	Auger electron spectroscopy
AFM	atomic force microscopy
CMA	cylindrical mirror analyzer
CNTs	carbon nanotubes
CVD	chemical vapor deposition
DFT	density functional theory
EBL	electron beam lithography
EDX/EDS	energy dispersive X-ray spectroscopy
GC	gas chromatograph
HDS	hydrodesulphurization
HREELS	high resolution electron energy loss spectroscopy
IF	inorganic fullerene-like nanoparticles
LEED	low energy electron diffraction
MBRS	molecular beam relaxation spectroscopy
MCS	Monte Carlo simulations
NDSU	North Dakota State University
NT	nanotubes
NP	nanoparticles
PNNL	Pacific Northwest National Laboratory
PVD	physical vapor deposition
SEM	scanning electron microscopy
STM	scanning tunneling microscopy
TEM	transmission electron microscopy
TiNTs	TiO_2 nanotubes
TDS	thermal desorption spectroscopy
TOF	time of flight spectroscopy
UHV	ultra-high vacuum
UPS	ultraviolet photoelectron spectroscopy
UV	ultraviolet
XPS	X-ray photoelectron spectroscopy

List of acronyms and abbreviations – scanning probe techniques

AFM	Atomic Force Microscope
PSTM	Photon Scanning Tunneling Microscope
SCM	Scanning Capacitance Microscope
NFTM	Near Field Thermal Microscope
SICM	Scanning Ion Conductance Microscope

TAM	Tunneling Acoustic Microscope
PCM	Point Contact Microscope
BEEM	Ballistic Electron Emission Microscope
IETS	Inelastic Electron Tunneling Spectroscopy

List of acronyms and abbreviations – nano-science

SLG	single layer graphene
MG	monolayer graphite
GO	graphene oxide
r-GO	reduced graphene oxide
HOPG	highly oriented pyrolytic graphite
Bucky paper	thick multi wall CNTs layers
CNFs	cup-stacked carbon nanofibers
CNTs	carbon nanotubes
SWCNTs	single wall carbon nanotubes
MWCNTs	multi wall carbon nanotubes
o-CNTs	open-end CNTs
c-CNTs	closed-end CNTs
BCNTs	bamboo-like carbon nanotubes
IF	inorganic Fullerene-like materials
NT	nanotubes
Peapods	C_{60} inside of NTs
TiNTs	TiO_2 nanotubes
Nanopipes	perhaps not so common but refers to CNTs with diameter larger than 100 nm
Au@TiNTs	Au nanoparticles on TiNTs, i.e., metals@NT

Useful web sites – internet resources

See PDF file on CD which has clickable links.

Reference data

http://www.unitconversion.org/unit_converter/pressure-ex.html

Historic notes

http://en.wikipedia.org/wiki/Irving_Langmuir

http://en.wikipedia.org/wiki/Svante_Arrhenius

Software, animations, tools

http://www.photon.t.u-tokyo.ac.jp/~maruyama/wrapping3/wrapping.html

www.jcrystal.com/products/wincnt/

Acknowledgement of images

 A few images of nanostructures were made with free software, see *"Nanotube Modeler"* www.jcrystal.com/products/wincnt/ (download 2010)