IUVSTA Workshop on
Nanostructure Characterisation by Electron Beam Techniques

IUVSTA71

Castle Hernstein, June 24-28, 2013

Programme Schedule and Book of Abstracts

Edited by
Wolfgang S.M. Werner, Mihaly Novak
and Cedric J. Powell

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Welcome

Welcome to the 71st IUVSTA workshop on nanostructure characterisation by means of electron beam techniques IUVSTA71 , in Castle Hernstein, June 24-28, 2013.
There is an increasing need for precise characterisation of nanostructured surfaces. While novel techniques have been introduced for this purpose in the recent past, the full potential of conventional surface analysis techniques employing electron beams for nanometrology is presently not exploited. The aim of the workshop is to improve quantitative understanding of the transport of electrons in nanostructures in order to widen the scope of nanostructure analysis and improve its accuracy. For this purpose, the workshop will highlight *the present state-of-the-art*, identify *the most urgent problems*, and provide a guideline for *future developments* on the following topics:

- Measurement and calculation of fundamental quantities needed for nanoscale calibration by means of electron beam attenuation.
- Influence of nanomorphology and manybody effects on electron transport.
- Optimisation of experimental approaches and quantitative data interpretation.

The workshop venue provides an ideal ambient for intensive discussion among the participants on the above topics and on the basis of the submitted abstracts, compiled in this book, it is to be expected that the workshop will provide a scientifically as well as socially exciting week. The IUVSTA71 organizing committee wishes all participants of the IUVSTA71 workshop a fruitful conference and an enjoyable stay in Castle Hernstein.

Wolfgang Werner
Chair of IUVSTA 71

Organizing Committee

C. Eisenmenger-Sittner	Finances
M. Marik	Workshop Office
M. Novak	Scientific Programme, book of abstracts
C. J. Powell	Scientific Programme
W.S.M. Werner	Chair

Contact

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fax:+43-1-58801-13499 (before IUVSTA71)

Invited Speakers

Hagai Cohen	IL	Near and far-field spectroscopy at the nano-scale using focused electron beams
Christian Colliex	F	Mapping the surface structural and electronic properties of individual nanoparticles with the tiny beam of a Scanning Transmission Electron Microscope (STEM)
Don Baer	US	Characterizing Nanoparticles for Environmental and Biological Applications
Dave Castner	US	Nanoparticles in Biomedical Applications: Characterization Challenges, Opportunities and Recent Advances
Shigeo Tanuma	JP	Calculations of Electron Inelastic Mean Free Paths in Solids Over the 50 eV to 30 keV Range with Relativistic Full Penn Algorithm
Rafael Garcia-Molina	ES	Inelastic scattering of proton beams in biological materials
Cesc Salvat-Pujol	D	Surface excitations in electron spectroscopy
Zhe-Jun Ding	CN	Roughness effect on electron spectrum
Cesc Salvat Gavalda	ES	Inelastic collisions of charged particles: PWBA and asymptotic Bethe formulas
Laszlo Kover	H	Intrinsic and surface excitations in XPS/HAXPES
Wolfgang Drube	D	Electronic characterization of nano-structured materials by HAXPES
Chuck Fadley	US	Characterization of Nanostructures with Hard X-Ray Photoemission
Mihaly Novak	H	Monte Carlo simulation of supersurface electron scattering effects
Alex Shard	UK	Practical XPS Analysis of Nanoparticles
Hideki Yoshikawa	JP	Energy loss functions and IMFPs derived by factor analysis of reflection electron energy loss spectra
Kyung-Joong Kim	KR	Traceable Thickness Measurement of nm Oxide Films by XPS
Alex Jablonski	PL	Quantification of XPS Analysis of Stratified Samples
David Liljequist	S	Model studies of the validity of trajectory methods for calculating very low energy (<100 eV) electron transport in condensed media
Maurizio Dapor	I	Monte Carlo simulation of secondary electron emission in the low-energy domain

The IUVSTA71 Dokuwiki:
an internet resource for the community by the community

An IUVSTA71-dokuwiki has been established with the aim of creating an internet resource of the field as one of the outcomes of the workshop. The purpose of this wiki is to provide a platform where all workshop participants can upload material they wish to share with their peers. Participants can use this portal to deposit datasets, software, comments, noteworthy results in the form of pictures, tables etc., along with contributions to ongoing discussions, in this way creating an ongoing discussion of the topic, accessible world-wide via the internet. The IUVSTA71 dokuwiki can be edited by the participants before, during and after the workshop. During the workshop, editing can be done on any of the computers located at the workshop office, or via personal laptops via the free WLAN which will be available during the workshop.

Invited speakers are requested to deposit their lecture notes on their personal section of the dokuwiki. Other participants are encouraged to do the same with their presentations (pdf- or ppt- files of their lecture or poster).

Navigating and editing the IUVSTA71-dokuwiki

We strongly encourage you to participate in this (experimental) project because we believe that it can become a valuable reference for the community to refer to after the workshop. Please feel free to contribute your presentation slides, papers, links to online-ressources, personal comments et cetera., keeping in mind that the final result will be **public**, implying that the contents should be **legal**, i.e. it should not contain any copyrighted material. The following section shall guide you through your first steps in the wiki.

Visit the wiki

`http://femto.iap.tuwien.ac.at/iuvsta71/`

The main page contains some very basic information and links which might be helpful if you have not used dokuwiki ever before.

Navigation

The sidebar allows you to navigate through the wiki. Expand the "users"-branch and click on your name to get to your own page, which is already created and waits to be filled with content.

Fill your page with content

In order to edit the page you can either click at the very top "Edit this page" to get to the editor where you will be able to include content. If you wish to modify a section within the page (e.g. "Presentation slides") only, click the "Edit" button associated with this section to get to the editor.

Uploading files

Uploading files can be done via the media manager. Once you are in the editor click the media-manager-button. In the panel to the left navigate to your namespace.

This is important to prevent that files get mixed up and everything stays well arranged. Subsequently, choose the files you wish to upload. Confirm the upload by clicking the corresponding button. Finally, you can click the file you wish to embed in your page and a link will appear at the current cursor position in the following form:

```
{{:users:yournamespc:your.file|<text to display> }}
```

Further information

For further information, please refer to the tutorial-page which you can easily navigate to using the sidebar.

Workshop Venue

The workshop will be held at Hernstein Castle, nowadays one of the most magnificent seminar hotels in Austria. This is a historic chateau once owned by the Habsburg family (Archduke Leopold Ludwig). Located in an idyllic park with a small lake it is just 50 km from Vienna city centre. Hernstein Castle is situated at the fringe of the Viennese Basin, in the stepped footland of the Styrian and Lower Austrian limestone alps. Its history goes back to medieval times: once the castle safeguarded the street to Berndorf Village and the valley before it. In former times the building comprised a housing unit and a chapel and could be seen from far away. It would have been very difficult to expand the building, therefore a new castle - the core of todays castle - was built in the valley at the foot of the mountain where the old castle had been built.

After the Turkish wars this new building was expanded and in the 18th century it got a uniform facade. For a long time the castle was owned by the Habsburgs and was used as domicile by archduke Leopold Ludwig. The renowned architect Theophil Hansen designed the castle - and thats how you will find it today.

Nowadays the Castle houses a luxurious seminar hotel with excellent meeting facilities, and modern hotel rooms with shower, toilet, TV etc. According to the motto “mens sana in corpore sano“ the hotel also offers a lot of physical activities and helps our guests to relax such as an indoor swimming pool, sauna, etc.
Address:
Seminarhotel Schloss Hernstein
Berndorfer Str. 32
A-2560 Hernstein, Austria
www.schloss-hernstein.at

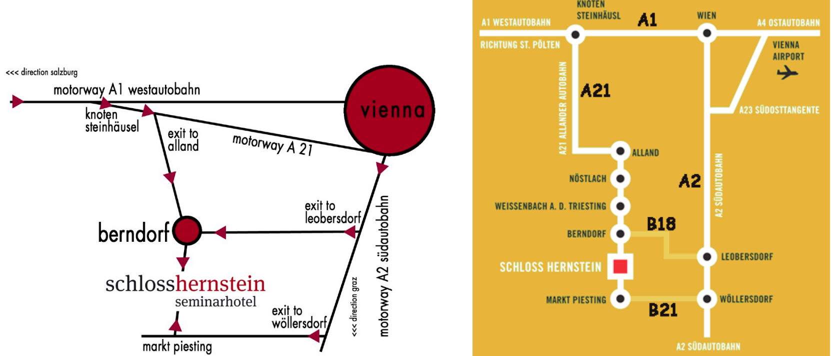
Arrival

- By Plane
  For participants arriving at Vienna International Airport (VIE) in Wien-Schwechat, we offer to organize a direct shuttle transfer to the workshop site in Hernstein on Monday, Jun. 24th, 2013. The shuttle busses (up to 4 persons) are operated by a private company, and you will be picked up in the arrival hall of the airport by the shuttle driver. The fee for this shuttle bus is 66.- Euro per transfer (max. 4 persons per transfer) payable in cash or by credit card directly with the chauffeur. If you want to use this shuttle transfer (60 km, approx. 1 hour transfer time), we need to know your exact arrival time, flight number and airline; please return the shuttle reservation form by e-mail to Mrs. Marik at marik@iap.tuwien.ac.at. Please notice that in order to reach the minimum number of persons per transport, you may have to wait for other flights to arrive. Solo-transports (e.g. if you are not arriving on Sunday) can be arranged, but will be considerably more expensive (please inquire). Transport back to the airport on Friday, June 28th will be

organized during the conference, with possibly even cheaper fares depending on the number of passengers per trip. As an alternative to the shuttle bus, you may take a train from the airport to Vienna and change there to a train to Leobersdorf (approx. 2 - 3 hours); see section on the arrival by train below.

- By Train
  The train station closest to Hernstein is Leobersdorf (15 km). Take a train from Vienna station Meidling in the direction Baden and get off the train at Leobersdorf. The web-page of the Federal Austrian Railways BB can help you in finding your train connection from any European city to Leobersdorf. From Leobersdorf train station it is a 30 minutes taxi ride (approx. 28 Euros) to Hernstein.

- By Car
  The maps below show you the best routes to Schloss Hernstein. When using the A2 Autobahn (motorway), take the exit at Leobersdorf, follow the signs to Berndorf along B18. Right in the center of Berndorf, at a big street junction, turn left, following the signs to Hernstein (approx. 8 km). If you are travelling along Autobahn A1, take the A21 Autobahn at Steinhäusl junction. Leave the A21 Autobahn at exit Alland and follow the signs through Nöstlach, Weissenbach and Berndorf to Hernstein. Schloss Hernstein is near the entrance of the small village of Hernstein on your left-hand side.



Weather

The weather near Vienna in June is usually warm (15°C lows, 20-30°C highs) and dry. Occasional precipitation is possible.

Insurance/Disclaimer

The organisers cannot accept any liability or responsibility for death, illness, or injury to the person or for loss of or damage to property of participants and accompanying persons which may occur either during or arising from the workshop. Participants are advised to make their own arrangements in respect of health and travel insurance.

Social Programme

Welcome Reception

Time: Monday, Sept. 24th, 17:00
Location: Habsburgersaal /MV on the first floor.

Conference Dinner

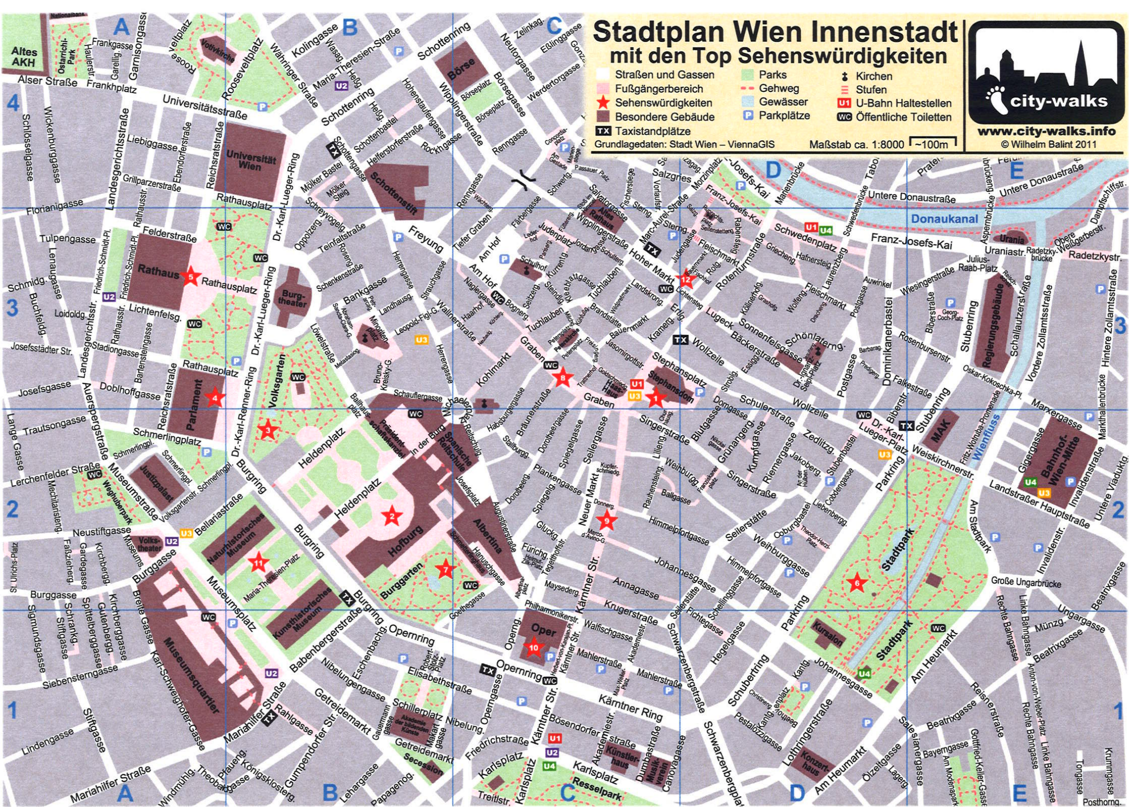
Time: Wednesday, June 26th, 19:00-22:00
Location: Heuriger Weiszbart, Leobersdorf
Departure by bus: 18:15 sharp in front of the hotel.

Free Sightseeing Tour Vienna City Centre for accompanying persons

An optional tour through the city of Vienna will be available on Tuesday, June 25th. A free shuttle for accompanying persons has been organised for a free sightseeing tour of the Vienna City centre. The bus will waiting by the hotel entrance at **8:45 AM** and will depart at **9:00 AM** sharp. The estimated time of arrival in Vienna (downtown Schwedenplatz) is **10:00 AM**

To start the sightseeing by Schwedenplatz visit e.g. the oldest church "Ruprechtskirche' (11th century), walk along Rotenturmstraße to the town's landmark "Stephansdom", Graben with the "pest pillar", walk along the Graben-Kohlmarkt you can find a lot of historical buildings e.g. "Hofburg with Sisi-Muesum, Imperial Treasury, Spanish Riding School", "Parliament", "city hall", "Justice palace", "Museum of Natural History", "Museum of Art History", and so on, Mariahilfer Straße strip mall, Krntner Straße strip mall, Opera, Karlsplatz with "Karlskirche", Technical University of Vienna or make a walk along the danube canal (Schwedenplatz). Try coffee and cake specialities in the "Biedermeier"-coffeehouse Heiner (Kärntner Straße), if you like ice cream we recommend the Salon on Schwedenplatz Fam.Molin-Pradel vis a vis your busmeeting point, for lunch with typical vienna cuisine try the city wine tavern Esterhazykeller (Harrhof 1: Graben-Naglergasse-left Harrhof) or the Ilona Stüberl (Bräunerstrasse 2: side street Graben) with hungarian cuisine, furthermore you find typical vienna sausage kiosk (side street Graben: Seilerstätte or behind the opera Alpertinaplatz), to buy typical Vienna chocolate specialities visit the Heindl (Kärntner Straße and Rotenturmstrae Strae).

Please find enclosed a city map downtown (Schwedenplatz D3). If you have further questions, please don't hesitate to contact Mrs Manuela Marik at the workshop office.



The Bus back to Castle Hernstein will be waiting at the arrival location (downtown Schwedenplatz) at **15:45 PM**. Departure time will be **16:00 PM**. Arrival in Hernstein castle is scheduled for **17:00 PM**

We wish you a nice trip and hope you will enjoy it.

Scientific Programme

Oral Presentations

Oral presentations have a duration of 15 min including discussion (30 min for invited talks). The lecture room has a Macintosh (running OSX) and a PC (running windows) prepared for projection using a beamer. You can also bring your own laptop and connect it to our system before the beginning of the session featuring your presentation. If you bring a file of your presentation instead (e.g. a powerpoint- or PDF-file) you should upload and test it well in advance of your presentation.

Poster Presentations

A poster session will be held on the first floor of the Castle in Habsburgersaal /MV on Tuesday afternoon. Poster panels are A0 in size. Posters can be mounted on Tuesday and must be removed at the end of the poster session by the presenting authors.

Programme 71st IUVSTA Workshop: Nanocharacterisation by Electron Beam Techniques

Tuesday June 25

8:30-9:00	Opening Address
	Session 1: Fundamentals: Inelastic scattering Session Chair: David Lilljequist
9:00-9:30	**Inelastic scattering of proton beams in biological materials** *Rafael Garcia-Molina* Universidad de Murcia, Murcia, Spain
9:30-10:00	**Calculations of Electron Inelastic Mean Free Paths in Solids Over the 50 eV to 30 keV Range with Relativistic Full Penn Algorithm** *Shigeo Tanuma* National Institute for Materials Science, Tsukuba, Japan
10:00-10:30	Coffee-break
	Session 2: Fundamentals: Inelastic scattering Session Chair: Juana Gervasoni
10:30-11:00	**Surface excitations in electron spectroscopy** *Cesc Salvat-Pujol* J.W.Goethe-Universitt, Frankfurt/Main, Germany
11:00-11:30	**Monte Carlo simulation of supersurface electron scattering effects** *Mihaly Novak* Institute of Nuclear Research of the Hungarian Academy of Sciences ATOMKI) Debrecen, Hungary
12:00-14:00	Lunch
	Session 3: Applications of models for electron scattering Session Chair: John Villarubia
14:00-14:30	**Electron Scattering with Rough Surfaces in Surface Electron Spectroscopy** *Zhe-Jun Ding* University of Science and Technology of China, Hefei, China
14:30-15:00	**Monte Carlo simulation of secondary electron emission in the low-energy domain. Application to the microelectronics.** *Maurizio Dapor* Fondazione Bruno Kessler, Trento, Italy
15:30-16:00	Coffee-break
	Session 4: Secondary (slow) Electrons Session Chair: Cedric Powell
16:00-16:15	**SEM Simulation Program for dimensional Nano-Metrology** *Carl Georg Frase* Physikalisch-Technische Bundesanstalt PTB) Braunschweig, Braunschweig, Germany
16:15-16:30	**Modeling Scanning Electron Microscope Measurements with Charging** *John Villarrubia* National Institute of Standards and Technology, Gaithersburg,USA
16:30-16:45	**Transmission Mode in the Scanning Electron Microscope at Very Low Energies** *Ilona Müllerova* Institute of Scientific Instruments of the ASCR, Brno, Czech Republic
16:45-17:00	**Plasmon resonant (e,2e) spectroscopy** *Gianluca DiFillipo* Dipartimento di Scienze and CNISM, Universit Roma Tre, Rome, Italy
17:00-17:15	**Near Field-Emission Scanning Electron Microscopy with Energy Analysis** *Danilo Andrea Zanin* Laboratory for Solid State Physics ETH Zürich, Zürich, Switzerland
17:15-17:30	**Local crystallographic information in Kikuchi patterns of backscattered electrons: experiments and simulations** *Aimo Winkelmann* Max-Planck-Institute of Microstructure Physics, Weinberg , Germany

Poster Session

17:30-19:00 Tuesday, June 25

Electron multiple inelastic scattering analysis in bulk carbon film
Alon Givon Department of Nuclear Engineering, Ben-Gurion University of the Negev, Israel

Utilizing Artificial Neural Networks for the Automation of Auger Spectra Analysis
Besnik Poniku Institute of Metals and Technology, Ljubljana, Slovenia

Influence of Rolling Technology Process on Electron Transport in steels
Evgeny Alekseevitch Deulin Bauman Moscov State Technical University, Moscow, Russia

Effects of sudden photo electron-hole pair creation on the induced surface plasmon excitations in cylindrical nanorods
Juana L. Gervasoni Bariloche Atomic Center and Instituto Balseiro, Bariloche , Argentina

Comparison of calculated and experimental spectra of plasmon excitation in single-walled carbon nanotubes probed using charged particles
Juana L. Gervasoni Bariloche Atomic Center and Instituto Balseiro, Bariloche , Argentina

Plasmon potential induced by an external charged particle traversing a solid surface in incoming and outgoing trajectories
Juana L. Gervasoni Bariloche Atomic Center and Instituto Balseiro, Bariloche , Argentina

Plasmon-enhanced secondary electron emission from copper phthalocyanine deposited on
Gianluca DiFillipo Dipartimento di Scienze and CNISM, Universit Roma Tre, Rome, Italy

Multi-walled carbon nanotubes irradiated by proton beams: An energy loss study
Isabel Abril Departament de Fsica Aplicada, Universitat dAlacant, Alacant, Spain

Signal Intensity Distribution in PAR-XPS from Rough Surfaces
Josef Brenner AC2T research GmbH, Wr. Neustadt, Austria

Electron inelastic mean free paths for cerium dioxide
Marcin Holdynski Mazovia Centre for Surface Analysis, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland

ARXPS - simulation and data analysis
Steffen Oswald IFW Dresden, Dresden, Germany

ARXPS on Surface Pre-Treatments for LiNbO3 SAW substrate
Uwe Vogel IFW Dresden-Institute for Complex Materials and TU Dresden, Institute of Materials Science, Dresden, Germany

Secondary-Electron Electron-Energy-Loss Coincidence Measurements on Polycrystalline Aluminum
Alessandra Bellissimo, Wolfgang S.M. Werner, Francesc Salvat-Pujol, Rahila Khalid, Mihaly Novak and Gianni Stefani Institut für Angewandte Physik, Vienna University of Technology, Wiednerhauptstraße 8-10/134, Vienna, Austria

Definition of arbitrary surface nanomorphologies in SESSA
Maksymilian Chudzicki, Wolfgang S.M. Werner ,Werner Smekal and Cedric Powell Institut für Angewandte Physik, Vienna University of Technology, Wiednerhauptstraße 8-10/134, Vienna, Austria

Wednesday June 26

Session 5: Transport Models for Nanostructures
Session Chair: Mihaly Novak

08:30-09:00 **Inelastic collisions of charged particles: PWBA and asymptotic Bethe formulas**
Cesc Salvat Gavalda Universitat de Barcelona, Barcelona, Spain

09:00-09:30 **Model studies of the validity of trajectory methods for calculating very low energy (<100 eV) electron transport in condensed media**
David Liljequist Department of Physics, Stockholm University, Stockholm, Sweden

10:00-10:30 Coffee-break

Session 6: Electron Microscopy and EELS
Session Chair: Ilona Müllerova

10:30-11:00 **Mapping the surface structural and electronic properties of individual nanoparticles with the tiny beam of a Scanning Transmission Electron Microscope (STEM)**
Christian Colliex Universit Paris Sud, Orsay, France

11:00-11:30 **Near and far-field spectroscopy at the nano-scale using focused electron beams**
Hagai Cohen Weizmann Institute of Science, Rehovot, Israel

12:00-14:00 Lunch

Session 7 :XPS on Nanostructures
Session Chair: Dave Castner

14:00-14:30 **Practical XPS Analysis of Nanoparticles**
Alexander G. Shard National Physical Laboratory, Teddington, UK

14:30-15:00 **Traceable Thickness Measurement of nm Oxide Films by XPS**
Kyung-Joong Kim Korea Research Institute of Standards and Science, Yuseong-gu, Rep. of Korea

15:30-16:00 Coffee-break

Session 8: Contributed Papers and Panel discussion
Session Chair: Don Baer

16:00-16:15 **Sample-Morphology Effects on XPS Peak Intensities: Estimation of Detection Limits for Buried Thin Films**
Cedric J Powell Materials Measurement Science Division, National Institute of Standards and Technology, Gaithersburg, USA

16:15-16:30 **Experimental Effective Attenuation Length for applications in Hard X-ray photoelectron spectroscopy**
German R. Castro SpLine Spanish CRG BM25 Beamline at the ESRF, Grenoble Cedex, France and Instituto de Ciencia de Materiales de Madrid-ICMM/CSIC, Madrid, Spain

Thursday June 27

Session 9: HAXPES
Session Chair: Laszlo Köver

08:30-09:00 **Characterization of Nanostructures with Hard X-Ray Photoemission**
Chuck Fadley Department of Physics University of California Davis, USA

09:00-09:30 **Electronic characterization of nano-structured materials by HAXPES**
Wolfgang Drube Deutsches Elektronen-Synchrotron, Hamburg Germany

10:00-10:30 Coffee-break

Session 10: XPS on Nanostructures
Session Chair: Alex Shard

10:30-11:00 **Intrinsic and surface excitations in XPS/HAXPES**
Laszlo Kover Institute of Nuclear Research of the Hungarian Academy of Sciences ATOMKI) Debrecen, Hungary

11:00-11:30 **Quantification of XPS Analysis of Stratified Samples**
Alex Jablonski Polish academy of sciences, Warsaw, Poland

12:00-14:00 Lunch

Session 11: Optical Data and Instrumental developments
Session Chair: Maurizio Dapor

14:00-14:30 **Energy loss functions and IMFPs derived by factor analysis of reflection electron energy loss spectra**
Hideki Yoshikawa National Institute for Materials Science, Tsukuba, Japan

14:30-15:00 **PHOIBOS 225 HV: High energy electron spectrometers with wide acceptance angle pre-lens**
Thorsten U. Kampen SPECS Surface Nano Analysis, Berlin, Germany

15:30-16:00 Coffee-break

Session 12: XPS and Applications
Session Chair: Chuck Fadley

16:00-16:15 **Combined nano-AES and EDS characterization of materials**
Muriel Bouttemy Institut Lavoisier, Universit de Versailles St-Quentin, Versailles cedex, France.

16:15-16:30 **Electron beam induced changes in Auger electron spectra for Lithium ion battery materials**
Martin Hoffmann IFW Dresden and TU Dresden, Dresden, Germany

16:30-16:45 **Electron scattering in graphene/copper system**
Petr Jiricek Institute of Physics, v. v. i., Academy of Sciences of the Czech Republic, Prague, Czech Republic,

16:45-17:00 **Surface characterization of ZnO and Ag loaded metal oxide nanotubes using spectroscopic techniques**
Agata Roguska Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

17:00-17:15 **Monte Carlo simulations of low energy electron in nanostructures**
Zine El Abidine Chaoui Laboratory of Optoelectronics and Compounds. University of Setif1. Algeria

Friday June 28

Session 13: Practical Aspects
Session Chair: Hagai Cohen

08:30-09:00	**Characterizing Nanoparticles for Environmental and Biological Applications** *Don Baer* EMSL Pacific Northwest National Laboratory, Richland, WA, USA
09:00-09:30	**Nanoparticles in Biomedical Applications: Characterization Challenges, Opportunities and Recent Advances** *Dave Castner* University of Washington Seattle, USA
10:00-10:30	Coffee-break
10:30-12:00	Session 14: Panel Discussion Moderators: Don Baer and Dave Castner
	Workshop Closing
12:00-14:00	Lunch

IUVSTA71 Abstracts
Tuesday, June 25

Inelastic scattering of proton beams in biological materials

Rafael Garcia-Molina,[1,*] Isabel Abril,[2] Pablo de Vera,[2]
Ioanna Kyriakou,[3] and Dimitris Emfietzoglou[3]

[1]*Departamento de Física – CIOyN, Universidad de Murcia, E-30100 Murcia, Spain*

[2]*Departament de Física Aplicada, Universitat d'Alacant, E-03080 Alacant, Spain*

[3]*Medical Physics Laboratory, University of Ioannina Medical School, 45110 Ioannina, Greece*

*corresponding author: rgm@um.es (Rafael Garcia-Molina)

The energy deposited by swift proton beams through inelastic scattering in biological materials (such as liquid water or DNA) is known to lead to the subsequent damage of the cellular constituents of living tissues. A detailed knowledge of this energy deposition is needed in radiation oncology to accurately deliver the prescribed dose to the tumor volume, whereas maximizing the sparing effect to the surrounding healthy tissue.

The main magnitudes (stopping power, energy loss straggling, mean excitation energy, mean energy transfer...) characterizing the energy loss of a proton beam in biological media are calculated by means of the dielectric formalism, with a suitable description of the target electronic excitation spectrum through the MELF-GOS (Mermin Energy Loss Function – Generalized Oscillator Strength) method [1]. The comparison of our calculations with available experimental data for liquid water shows a satisfactory agreement.

To calculate the spatial distribution of the energy deposited by the proton beam, as well as the evolution of its energy and geometrical dispersion we use the SEICS (Simulation of Energetic Ions and Clusters through Solids) code [2], which combines Molecular Dynamics and Monte Carlo techniques to follow in detail the trajectory of each projectile, taking into account the main interactions between the projectile and the target constituents, as well as its dynamically changing charge-state. The simulated depth-dose curve shows an excellent agreement with the available experimental data.

References

[1] I. Abril, R. Garcia-Molina, C. D. Denton, F. J. Pérez-Pérez, and N. R. Arista, Phys. Rev. A **58** (1998) 357; S. Heredia-Avalos, R. Garcia-Molina, I. Abril, and J. M. Fernández-Varea, Phys. Rev. A **72** (2005) 052902.

[2] R. Garcia-Molina, I. Abril, S. Heredia-Avalos, I. Kyriakou, and D. Emfietzoglou, Phys. Med. Biol. **56** (2011) 6475.

Acknowledgments: We thank the European Regional Development Fund and the Spanish Ministerio de Economía y Competitividad (Project FIS2010-17225), as well as the COST Action MP1002 Nano-IBCT. PdV thanks the Generalitat Valenciana for a grant under the VALi+d program.

Calculations of Electron Inelastic Mean Free Paths in Solids over the 10 eV to 200 keV Energy Range with the Relativistic Full Penn Algorithm

H. Shinotsuka,[1] S. Tanuma,[2,*] C.J. Powell,[3] and D. R. Penn[3]

[1]*Advanced Algorithm & Systems, Co. Ltd., Ebisu 1-13-6, Shibuya, Tokyo 150-0013, Japan*

[2]*National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan*

[3]*National Institute of Standards and Technology, Gaithersburg, MD 20899, USA*

*Tanuma.Shigeo@nims.go.jp

The inelastic mean free path (IMFP) is an important parameter in XPS and other electron spectroscopies. Our initial IMFP calculations were made for 27 elemental solids, 15 inorganic compounds, and 14 organic compounds at electron energies between 50 eV and 2 keV. In recent years, there has been growing interest in XPS and related experiments performed with X-rays of much higher energies for both scientific and industrial purposes. We have therefore calculated IMFPs for electron energies up to 30 keV. Results have been reported for 41 elemental solids [2], and similar calculations for a larger group of inorganic compounds are in progress. There is also a need for IMFPs in transmission electron microscopy, and we have begun IMFP calculations for energies up to 200 keV.

We have calculated IMFPs for 41 elemental solids and 30 semiconductors at equal energy intervals on a logarithmic scale corresponding to increments of 10% from 10 eV to 200 keV. These calculations were made with optical energy-loss functions (ELFs) using the relativistic full Penn algorithm (FPA). The ELFs for semiconductors were obtained from first-principles calculations with the WIEN2K and FEFF codes from1 eV to 1 MeV.

Our calculated IMFPs could be fitted to a modified relativistic Bethe equation for inelastic scattering of electron in matter for energies from 50 eV to 200 keV. The average root-mean-square (RMS) deviation in these fits was 0.8% for the 41 elemental solids. The new IMFPs were also compared with IMFPs from the predictive TPP-2M equation [1] that was modified to include relativistic effects; the average RMS deviation in these comparisons was 11.9% for the 41 elemental solids and for energies from 50 eV to 200 keV. This average RMS deviation is almost the same as those found in previous similar comparisons for the 50 eV to 2 keV [1] and 50 eV to 30 keV ranges [2].

In the talk we will show comparisons of the new IMFPs and those calculated from Mermin model ELFs. We will also show the effect of the Born-Ochkur exchange correction on the FPA model.

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Surface excitations in electron spectroscopy

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A quantitative understanding of electron spectra relies on an adequate description of electron energy losses taking place both in the bulk of the solid and in the vicinity of the solid-vacuum interface (at either side of the surface). Several models for electron energy losses near planar interfaces have been published in the last three decades based on the semiclassic dielectric formalism (see references in [1]). However, these models often include several simplifying approximations: some are valid for selected trajectories, others employ a simplified dielectric response of the solid, etc.

A detailed model for surface excitations in electron spectroscopy has been derived within the semiclassic dielectric formalism, encompassing other models in the literature and allowing one to investigate their relevant physical assumptions. The model has been implemented in a Monte Carlo simulation of reflection-electron-energy-loss spectra (REELS). REELS have been simulated for 17 metals, obtaining a good agreement with published experimental spectra in absolute units (typically within ~10 \%).

The model has been further employed to interpret a series of recent electron energy-loss experiments. On the one hand, it has been instrumental in exposing the role played by surface excitations in secondary-electron emission in a recent measurement of a double-differential secondary-electron yield from polycrystalline samples (Al, Si, Ag) employing a time-coincidence technique. On the other hand, it has been used to interpret a series of angle-resolved REELS of a Au surface at grazing incidence [2]: it has been shown that energy losses at the vacuum side of the interface constitute an essential contribution to electron energy-loss spectra and must be accounted for in detail for a quantitative understanding of REELS.

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Monte Carlo simulation of supersurface electron scattering effects

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Supersurface electron scattering, i.e. electron energy losses and associated deflections in vacuum above the surface, was investigated by Monte Carlo simulation in reflection electron energy-loss (REELS) setup. These theoretical calculations predicted a strong structure in the detected supersurface inelastic scattering probability that was proven by experiments in case of Au sample leading to the unambiguous identification of the vacuum side electron scattering in reflection experiments [1]. These deflections, in vacuum side surface plasmon excitations, can establish a link between the detected vacuum side surface loss intensities and the differential elastic scattering cross section (DECS) resulting in the observable structure. The details and consequences of this supersurface electron scattering will be presented together with a Monte Carlo simulation study on the energy, geometry and material dependence of these complex phenomena.

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Monte Carlo simulation of secondary electron emission in the low-energy domain. Application to the microelectronics.

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Monte Carlo (MC) technique permits solving mathematical and physical problems of great complexity. Transport MC allows predicting the behavior of charged particles traveling through the matter. It has been widely used, in particular, to solve microelectronics problems. In this work, transport MC simulations concerning secondary electron emission are applied to (i) the study of image contrast in silicon *p-n* junctions [1] and (ii) to the calculation of line-scan of resist materials (e.g. PMMA) with given geometrical cross-sections deposited on silicon substrates [2]. Theoretical results are validated through a comparison with the available experimental data.

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Electron Scattering with Rough Surfaces in Surface Electron Spectroscopy

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Surface topography influences the signal intensity in a surface electron spectroscopy, such as XPS, AES, EPES and REELS through modulation of frequency of electron elastic scattering and inelastic scattering events. In order to quantify such an influence, it is necessary to study the role of the surface roughness effect on electron signals during their transport and emission near surface region. But it is difficult to deal with the surface roughness effect theoretically in a general form because the practical sample may present various kinds of surface topography structure which prohibits from a general mathematical modeling of structure. There is still little theoretical work dealing with the surface roughness effect in surface electron spectroscopy. Such a work is required to predict surface electron spectroscopy accurately, providing an understanding of the experimental phenomena observed [1,2]. In this work, we use a finite element triangle mesh method to build a full 3D rough surface model based on the surface topography measured by atomic force microscopy image [3]. Then Monte Carlo simulations of surface excitation have been performed for these rough surfaces. The simulation of REELS spectra and EPES spectra is found to agree well with the experiments and explain qualitatively the roughness effect [3,4]. In order to describe quantitatively the surface topography effect, surface roughness parameter (SRP) and roughness dependent surface excitation parameter (SEP) are introduced. SRP parameter is defined as the ratio of elastic peak intensities between a rough surface and an ideal planar surface, which describes the influence of surface topography on the elastically backscattered electrons; while SEP parameter describes the influence to electron inelastic scattering for surface excitation in surface electron spectroscopy. Calculations of SRP and SEP have been performed for several material surfaces with different surface roughnesses.

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SEM Simulation Program for dimensional Nano-Metrology

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The Scanning Electron Microscope (SEM) is a valuable and versatile instrument for imaging and characterisation of nanostructures. However, prerequisite for the application as a quantitative dimensional measurement tool is a proper calibration of the instrument and a physical model of SEM image formation that definitely correlates the SEM signal profile with the underlying specimen topography [1].

Here, we present the SEM simulation program MCSEM which models the different stages of SEM image formation and generates SEM grey level images of complex shaped nanostructures. The individual aspects of image formation are implemented in different modules of the program, i.e. the electron probe formation, the three-dimensional specimen model, the electron probe – solid state interaction, the emission of secondary electrons, electric fields and the dynamic charge-up behaviour of the specimen as well as secondary electron ray-tracing in the vacuum above the specimen surface, and different detector models.

The Monte Carlo simulation of electron diffusion in solid state is the core of the program. It is based on tabulated elastic Mott scattering cross sections by Salvat and Mayol [2] and the Bethe continuous slowing down approximation in the modification of Joy and Luo [3]. The three-dimensional specimen model is realized by methods of constructive solid geometry (CSG), combined with the possibility to include two-dimensional height maps. The electric field is calculated using finite element methods (FEM). The model includes space charge in dielectrics due to absorbed primary electrons, emitted and reabsorbed secondary electrons, as well as metals on a floating or fixed potential. A secondary electron ray-tracing algorithm models the SE trajectories in the electric field. Dynamic charge-up behaviour can be modeled in a feedback loop, involving an iterative series of field recalculations. Detector models comprise an InLens SE detector based on electron-optical detector efficiency calculations plus BSE and Transmission SEM (TSEM) detectors [4].

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Modeling Scanning Electron Microscope Measurements with Charging

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Nanostructured samples that are relevant in semiconductor electronics manufacturing or in nanotechnology are often comprised of mixed materials, some of which are insulators. Accumulated charges in insulating regions exposed to the electron beam or to scattered electrons generate electric fields that alter the contrast and positions of features in acquired images. To interpret the images it is necessary to account for these effects.

For this purpose, the existing JMONSEL [1,2] simulator has been augmented with charging-related modeling capabilities. JMONSEL already performed Monte Carlo scattering simulations that included elastic scattering via the Mott cross sections, inelastic scattering via the dielectric function theory approach (when the requisite material data are available), phonon scattering, and electron refraction at material boundary crossings. For simulations in which charging is important, the sample is represented as a tetrahedral mesh with variable mesh size: fine in the region of interest and increasingly coarse with distance (Fig. 1). The net charge due to trapped electrons or holes in each mesh element is tracked. Simulation proceeds iteratively in a cycle that includes finite element solution of the electric fields followed by a scattering phase with electron transport modified by the electric field.

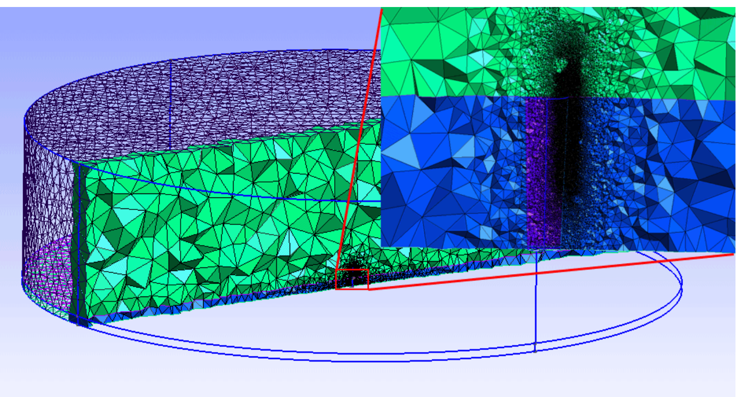

Fig. 1. Cutaway of meshed contact hole and surrounding volume. Tetrahedra that intersect a plane through the axis of the hole are rendered as solids. Oxide is blue, the vacuum above the hole is green, and (inset) the vacuum in the hole itself is purple.

The new capabilities have been used to simulate imaging of unfilled contact holes with radius 35 nm to 70 nm through SiO_2 (Fig. 1) with a view to determining the dependence of visibility of the hole bottom upon hole size and imaging conditions. Results indicate that under appropriate conditions, the SiO_2 develops a beneficial positive surface potential that saturates at a scan-size dependent amount. This potential helps to extract electrons from the hole bottom.

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Transmission Mode in the Scanning Electron Microscope at Very Low Energies

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The Cathode Lens principle when implemented in the scanning electron microscope [1] enables us to operate from tens of keV down to zero landing energy at a high lateral resolution. Nowadays, resolutions of 0.5 nm at 15 keV, 0.8 nm at 200 eV and 4.5 nm at 20 eV are experimentally available [2]. Two segmented detectors are used for collection of reflected (BSE) and transmitted (TE) electrons. Examples of imaging of the graphene flakes in various collected signals are shown in Figure 1. Increase in the electron transmittance is expected at energies below 50 eV because of extending inelastic mean free path so the image contrast becomes based on another types of the collisions, see arrow in Figure 1d. The maximum transmittance of the single graphene layer was measured at 5 eV and data were compared with the results obtained by Raman spectroscopy [3]. The method can be useful for a new type of reflection spectroscopy, for examination of biological crystals, ultrathin tissue sections, etc. [4].

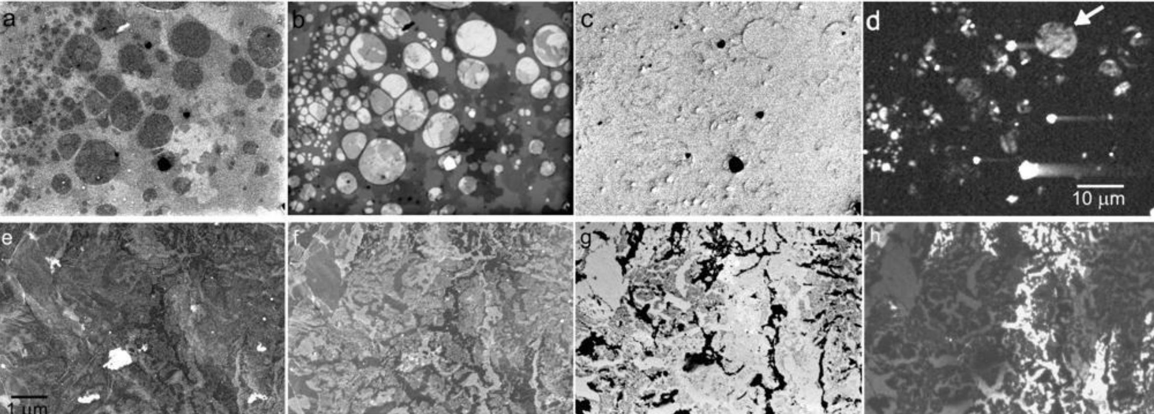

Figure 1. Micrographs of two graphene samples. Upper row: commercially available sample of the CVD graphene™, BSE at 3 keV (a), TE at 3 keV (b), BSE at 4 eV (c), and TE at 4 eV. Bottom row: exfoliated sample, BSE at 5 keV (e), BSE at 1 keV (f), TE at 500 eV (g), and TE at 20 eV (h).

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Plasmon resonant (e,2e) spectroscopy

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The (e,2e) process has been largely used to investigate ionization mechanisms and electronic structure in atoms, molecules and solids. In solids, one of the most efficient channels of electron impact energy transfer is excitation of volume or surface plasmons (collective excitations of the electron gas). Two main plasmon decay mechanisms have been foreseen: the excitation of nearly free secondary electrons and the excitation of pair of correlated free electrons[1]. In competition with these two channels, the ejection of a secondary electron due to direct scattering within a medium described by its inverse dielectric function has been proposed[2].

To establish the relative relevance of these secondary electron generation channels is of importance in many branches of fundamental and applied science.

In this paper will be reviewed (e,2e) plasmon assisted experiments performed on Al and Be clean surfaces. The early experiment on Al[3] , performed at 100eV incident energy, proposes that observed secondary electrons are emitted via a mechanism similar to photoemission with plasmon decay playing the role of photon absorption. The experiment performed always on Al at 500 eV[4] proves that surface plasmon decay accounts for roughly a quarter of the secondary electron spectrum. More recent experiment on Be[5] point to plasmon resonant (e,2e) processes as a relevant channel for secondary electron generation and for building a resonant momentum spectroscopy.

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Near Field-Emission Scanning Electron Microscopy with Energy Analysis

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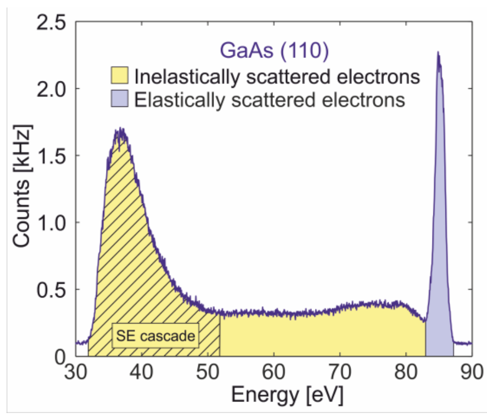
Based on the topografiner technology [1], Near Field-Emission Scanning Electron Microscopy (NFESEM) [2] uses low energy electrons, emitted from a polycrystalline tungsten tip via electric field assisted tunneling, to probe the target surface. The primary electron beam scatters at the surface generating secondary electrons, which are sampled by a suitable secondary-electron detector placed in the vicinity of the tip-sample junction. Currently, NFESEM technique is capable to resolve the topography of metals and semiconductors with nanometer lateral resolution. Moreover, preliminary studies on a W(110) surface covered by few monolayers Fe evidenced a chemical contrast arising from the different secondary-electron yields of Fe and W.

Here, we report on recent efforts of implementing energy analysis of secondary electrons into the NFESEM technique. The figure shows the energy spectrum of the electrons backscattered from a GaAs(110) surface. The typical overall shape of the secondary-electron spectrum testifies that both the elastically scattered and secondary electrons originate from the tip-specimen interaction zone. Taking into account the spatial resolution intrinsic to NFESEM we anticipate the technical feasibility of electron spectroscopy with a few nm spatial resolution. In addition, the presence of a sizeable amount of true secondary electrons opens the possibility of spin-polarized analysis of magnetized surfaces. [3]



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Local crystallographic information in Kikuchi patterns of backscattered electrons: experiments and simulations

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Important structural information from crystalline samples is provided by spectroscopic measurements of diffraction patterns of quasi-elastically backscattered electrons. To describe the diffraction of quasi-elastically backscattered electrons (BSE) with incident primary beam energies in the keV energy range, we use simulations based on the Bloch-wave approach of dynamical electron diffraction theory [1]. Details on the depth- and energy distribution of electrons leading to Kikuchi pattern generation are analyzed by Monte Carlo (MC) simulations of the BSE energy spectrum applying approaches from reflection energy loss spectroscopy (REELS) [2]. By experimental spectroscopic measurements from Silicon at 30kV, we show how inelastic scattering events are affecting the diffraction effects. Most notably, we demonstrate that inelastically scattered electrons can show more diffraction contrast than elastically scattered electrons [3]. High-resolution electron spectroscopy allowed us to resolve element-specific recoil effects in sapphire Al_2O_3 which in turn give rise to site-specific Kikuchi patterns for Al and O [4]. This provides a new way for local crystallographic analysis using backscattered electrons, potentially with nanoscale resolution in the scanning electron microscope.

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Multi-walled carbon nanotubes irradiated by proton beams: An energy loss study

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The irradiation with energetic proton beams impinging normal to the axis of a multiwalled carbon nanotube (MWCNT) is studied both experimental and theoretically, in the keV energy range. The MWCNTs are dispersed on top of a very thin film of holey amorphous carbon (a-C) substrate. Measurements of the proton energy loss distribution at the forward direction are performed by the transmission technique, obtaining energy loss spectra with two well differentiated peaks.

A semi-classical simulation is employ to elucidate the origin of the peaks in the energy distribution. The simulation follows the trajectories of each projectile by solving its equation of motion, where the electronic stopping force was accounted for by a non-linear density functional formalism depending on the local electronic density.

By the simulation we predict that the experimental low-energy-loss peak is due to protons moving in quasi-channelling between the most external walls of the MWCNTs. The experimental high-energy-loss peak are those channelled protons, with larger impact parameter and small angular dispersion after traversing the a-C film, which can reach the detector at zero angle with only an extra energy loss that shifts to a lower energy their energy distribution [1].

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Secondary-Electron Electron-Energy-Loss Coincidence Measurements on Polycrystalline Aluminum

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The double-differential secondary electron-electron energy loss coincidence spectrum of Al has been measured for 100 eV primary electrons and energy losses between 0–25 eV. This energy loss range comprises the simple scattering regime of energy losses and therefore allows one to gain unique insight in the creation of secondary electrons (SE) in the course of excitation of single surface and bulk plasmons in Al.

The experiment was performed in a UHV-system containing a hemispherical mirror analyser (HMA) for the detection of the fast backscattered electrons and a time-of-flight (TOF) spectrometer with an acceptance angle of approximately 2π for the slow secondaries, which are detected in coincidence with the backscattered primaries.

The acquired double-differential coincidence spectra show very specific regions corresponding to different excitation processes. In the low-energetic loss region - between the work function delimitation and the bulk plasmon energy – the energy losses can be entirely attributed to surface excitations, where also contributions of super-surface scattering can be identified.

At the energy loss corresponding to the bulk plasmon excitation, a sudden and unexpected transition can be observed, leading to a decrease of intensity. This is due to the increment of depth range where the SE are emitted from. The region beyond the bulk plasmon characteristic energy loss is dominated by the multiple inelastic scattering regime. The remarkable similarity of coincidence TOF-spectra for the energy loss range 0–25 eV with the single TOF-spectra shows that the main difference in the cascade regime is caused by the multiple excitations of bulk plasmons. Consequently, through the analysis of the SE spectrum measured in coincidence with surface and bulk plasmon losses a much more detailed picture concerning the contribution of plasmon decay to the emission of secondaries can be attained.

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Signal Intensity Distribution in PAR-XPS from Rough Surfaces

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One limiting factor in quantitative Angle Resolved X-Ray Photoelectron Spectroscopy (AR-XPS) is the difficulty of interpreting measured data in case of inhomogeneous chemical composition, morphology and topography. The determination of layer thicknesses and the underlying understanding of signal generation, for example, are prone to large uncertainties.

This contribution deals with the impact of surface roughness in parallel AR-XPS (PAR-XPS) measurements. In order to study this, a layered structure, laterally uniform in both chemical composition and layer thickness, covering the overall topography was chosen.

For sake of simplicity, a well-defined periodic roof-like surface was considered and compared with a flat one, which allows one to validate the computational results by an analytical closed form. In particular, PAR-XPS measurements and the corresponding numerical investigations were performed on a silicon sample covered by a native oxide layer, containing both a parallel roof-like topography and a flat surface area. The sample topography was measured by Atomic Force Microscopy (AFM) and parameterized using Non-Uniform Rational B-Splines (NURBS) [1]. This parameterization is general enough giving the possibility to be extended to arbitrary rough surfaces as characterized by well-known metrological methods. Another advantage of NURBS is the intrinsic availability of arbitrary small surface facets and the fact that it directly provides the angular orientation of these facts with respect to a fixed global coordinate system.

For each NURBS-facet the contribution to the total PAR-XPS intensity was calculated using a generalized Beer-Lambert law in straight line approximation by also taking into account the shadowing due to roughness of the surface. The computational results were cross-checked for a nominally flat surface using the SESSA [2] simulation toolkit.

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Definition of arbitrary surface nanomorphologies in SESSA

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The NIST database for quantitative Auger-electron and X-ray photoelectron spectroscopy SESSA is a very functional software tool capable of simulating AES and XPS spectra for a given instrumental setup and a number of predefined geometries. Currently it is possible to simulate planar, layered samples, islands and spheres on layered specimen as well as layered spheres on uniform substrates.

The PENGEOM geometry package provides a very flexible and versatile set of tools allowing to define arbitrary geometries for Monte Carlo simulations as well as tracking the movement of the particle of interest within the geometry. The geometry definition is based on the use of fuzzy quadric surfaces, which minimizes the impact of round-off errors as well as keeps the mathematical complexity down since the intersection of a ray with the border of a material specified by a quadric surface can be determined by calculating the discriminant of the particular quadratic equation.

SESSA has been extended to be able to deal with arbitrary surface nanomorphologies using PENGEOM, which can be defined by a user by means of the PenGeom-Viewer made available within the PENGEOM package.

As an example a deep-buried nanostructure measured with HAXPES will be presented.

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Influence of Rolling Technology Process on Electron Transport in steels

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The author's results of steel samples investigation with Electron Microscopy and Secondary ION Mass Spectrometry are presented. They help us come to new conclusions about the results of friction processes which lead to the steel samples destruction at traditional friction and rolling friction processes. It was shown that the sample micro structure forming process linked with hydrogen molecules penetration into sample, that influences on the steel properties according the "dry friction" theory[1].

The experiments task was consider the results of friction processes which lead to the steel samples destruction at traditional friction and in steel sheets rolling technology processes. It was shown that the sample micro structure forming process coincides with hydrogen molecules penetration process that influences on the steel properties according "dry friction" theory. The first experiments were done with Secondary ION Mass Spectrometry (SIMS) usage, as it is known, that SIMS analysis allows measurements of concentration of dissolved gases including H_2 and D_2 with high accuracy and the method help authors to predict [1] and then to discover [2] the role of dry friction in the process of hydrogen isotopes dissolution that raises the hydrogen isotopes concentration in steel up to catastrophically high level. The first experiment was done in vacuum chamber at Deuterium pressure P_{D2}=1x10^{-1} torr and the experimental results on Fig.1 show, that the deuterium concentration into the samples (ball bearing elements) after 0,2- 2 min of friction process increases 2000 times at the depth 0,1-0,2 microns. We can see that the deuterium atoms concentration is close to C_{D2}=2x10^{19} at/sm^3, that is rather more and contradict to figures of Sieverts equation, and in future it leads to the hydrogen illness of the metal in the volume near the surface .

The main task of the experiment was to estimate the sheets rolling process influence on sheet's metal mechanical properties. The initial results were received with SIMS analysis and show [3], that "hydrogen illness" of the mechanical elements and their destruction are the result of hydrogen dissolution at friction in rolling processes. It was shown above, the SIMS analysis was used because it helps to detect the concentration of gases at analysis adequacy about 0,0001%, including H_2 and D_2 at the depth not more then 1-10 mic.

The main experiment was done in frames of converter steel melt on Azov Steel Co plant. (Ukraine)..The samples cited from steel sheet, heated till 1000-1100°C and 1250°C, and then were cooled by room air or sand The experiments of Ikonnikova E.I. with the electron microscope (Russian made УЭМВ100К) show, that the plastic properties of the metal deterioration as a result of deformation may be seen as the results of sulfide inclusions and its hydrogen environments transformation at sheets rolling process we can see on Fig.1a – Fig1b. where the initial form of sulfide particles (black, Fig.1a) transformation into "roundish" form particles(Fig.1b),.may be explained as a result of hydrogen diffusion out of sulfide zones, which we consider as a "limited sources of hydrogen" and then the hydrogen concentration becomes less and the sheet's mechanical properties become better.

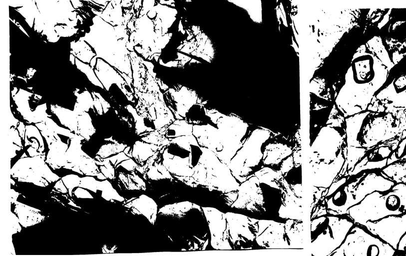
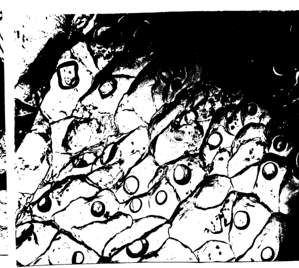

Fig.1a(left).Sheet (scale x 4000) of steel after heating 1150 ^{o}C before rolling, dark areas (Fe-Mn)-S zones, correspond to weak steel mechanical

Fig.1b.(right) The same sheet (scale x 3200) of steel after heating 4hours55min at 1250^0 C, shows the globular formations appearing, corresponding to steel parameters increasing (Ikonnikova result, Azov Steel Co)

The experiment's task was to see the process of hydrogen atoms diffusion results from the "limited sources» as it shown above. In a role of "limited sources" was the steel sample, which surface was covered with one monolayer (0,35 more correct figure) of heavy water . The results shows that deuterium initial concentration distribution decreasing 10 times near the surface and increasing 25 times at the depth 0.3- 4.5 microns from the surface after diffusion from the limited source. So we can see, that near the surface ("limited sources") where the initial deuterium atoms concentration was C_{0D} = 10^{22} at/sm^3 this concentration decreases till C_{0D} = 10^{18} at/sm^3 that shows, that the hydrogen illness was removed, and our patient (steel sheet) comes to "good health". From the another side the hydrogen atoms concentration increases near the rolls and sheets surfaces after the sheets rolling the initial hydrogen atoms concentration in sheet steel C_H = 10^{17} - 10^{19} at/sm^3 increases till C_{0H} = 10^{23} at/sm^3 at the depth 0,1 - 3,5 mm after 3-5 minutes rolling process. It shows, that the "hydrogen illness" comes from the surfaces into the sheet's and roll's steel at rolling technology realisation.

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Effects of sudden photo electron-hole pair creation on the induced surface plasmon excitations in cylindrical nanorods

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In this work we study the effect of the excitation of surface plasmons in a metallic cylindrical nanorod by a suddenly created electron-hole pair, using a classical model for the emerging electron and a quantum-mechanical model for the plasmon field in the cylinder [1]. The emitted electron and the hole interact independently with the free electrons in the metallic Al, generating electron density oscillations. Two different trajectories for the emerging electron (parallel to the axis and radial) are studied in an aluminum nanorod. The average number of excited plasmons indicates how important the role of the hole in the excitation process is. We found that the results can be very different according to the trajectory of the emerging electron. We also found that the separation of the intrinsic and extrinsic process is sometimes not applicable.

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Comparison of calculated and experimental spectra of plasmon excitation in single-walled carbon nanotubes probed using charged particles

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We study the excitation of plasmons due to the incidence of a fast charged particle that passes through a single-wall carbon nanotube. We use a quantized hydrodynamic model, in which the sigma and pi electron systems are depicted as two interacting fluids moving on a cylindrical surface [1]. Calculations of the average number of the excited plasmons and the corresponding energy loss probability for the swift electrons are compared with several experimental results for electron energy loss spectra recorded using transmission electron microscopes. We are able to identify the sigma and pi plasmon peaks and elucidates the origin of various spectral features observed in different experiments.

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Plasmon potential induced by an external charged particle traversing a solid surface in incoming and outgoing trajectories.

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In this work we study the movement of an external charged particle traversing a solid surface, and coupling with the bulk and surface plasmon excitations. We pay special attention to the differences and similarities between incoming and outgoing trajectories [1], finding some novel oscillatory structures that can be ascribed to interference effects between direct and reflected contributions.

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Electron multiple inelastic scattering analysis in bulk carbon film

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Hard x-ray photoelectron spectroscopy (HAXPES) is a powerful emerging instrument in the field of surface analysis. It extends the photoelectron energy range analysis up to 15,000 eV and opens the possibility to study much thicker films, buried layers, and bulk electronic properties. When analyzing thin films, some of the electrons loss energy through inelastic processes and as a result the signal electron is attenuated. However, these electrons still appear in the lower part of the spectrum and have a screening effect on the desired signal electron. Extensive work was carried out over the years in order to strip the attenuated electrons from the signal electron peak. The main process that gives rise to attenuated electrons at the measured spectrum is the multiple inelastic collisions (MIC) in the bulk material. As the measured film gets thicker, the MIC effect intensifies up to a point where the signal electron is under the detection limit. Currently, only the signal electron in the HAXPES spectrum is analyzed.

We present a new approach that uses the attenuated part of the electron spectrum. In this method, the attenuated part of the electron HAXPES spectrum is treated as a whole to calculate the average electron energy loss. The average electron energy loss is the result of inelastic collisions in the material and hence, conveys information about the electron transport process. Careful analysis of the measured energy loss can provide new ways for measuring IMFP at high energies.

Nanometeric carbon layers deposited over copper and silicon substrate were used to test this approach at the Spanish beam-line (Spline) in the European synchrotron radiation facility (ESRF). The measured results demonstrated the unique structure of the MIC spectrum, and showed good agreement with the predictions of the multiple inelastic scattering theory.

Electron inelastic mean free paths for cerium dioxide

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Among semiconductor materials, a wide band gap semiconducting oxide like cerium dioxide (CeO_2) has attracted considerable interest due to their structural, chemical, electrical and optical properties. Especially important are surface properties of this binary semiconductor for photo- and heterogeneous catalysis. However, the accurate quantification of surface analyses using AES and XPS requires the knowledge of the inelastic mean free path (IMFP) values for CeO_2, which are still unavailable. In this work, we evaluated the IMFP in cerium dioxide from the relative elastic-peak electron spectroscopy (EPES) measurements.

Nanocrystalline CeO_2 pellet was examined. Prior to XPS-EPES measurements, the sample was sputter-cleaned and amorphized by 0.5 keV Ar^+ ions. Its surface composition was determined by XPS using a Thermo Scientific Microlab 350 spectrometer. Relative EPES measurements (Ni and Au standards) for electron energies 0.5-2 keV were performed using the same spectrometer with a spherical sector analyzer. During the measurements, the electron gun was located at the normal to the surface and the analyzer axis was located at 60° to the surface normal. The acceptance half-angle of the analyzer was 6°.

Cerium dioxide sample were analyzed by XPS after 0.5 keV argon ion etching. As obtained from the XPS multiline analysis [1], the composition of the CeO_2 surface was close to stoichiometric composition. The IMFP data evaluated from the relative EPES were uncorrected for surface excitations and compared with those calculated from the predictive TPP-2M formula [2]. The IMFPs measured and calculated for CeO_2 are shown in Table 1. Good agreement was found between the measured and calculated electron IMFPs in CeO_2.

Table 1 Values of measured and predicted IMFPs (in angstroms) for CeO_2

Energy (eV)	EPES (Ni standard)	EPES (Au standard)	TPP-2M [2]
500	8.0	10.8	11.2
1000	15.1	15.8	18.5
1500	22.9	25.3	25.2
2000	35.8	37.0	31.5

Acknowledgements

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ARXPS - simulation and data analysis

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Thin film technology developments require both reliable thin-layer and interface characterization. A non-destructive method often used for depth-profile characterization in the nm thickness range is the angle-resolved X-ray photoelectron spectroscopy (ARXPS). However, to extract the in-depth information from such measurements in practice, dedicated mathematical models have to be applied. A further limitation is that commonly the use of ARXPS is restricted away from the near-surface measuring angles due to effects of elastic scattering on the measured intensities in this region. A further major point is the well-accepted restriction that the information content of the ARXPS measurements should not be overvalued [1].

In this context the paper discusses the following topics:
(I) A procedure for computer simulation of reliable ARXPS data for complex near-surface structures considering elastic scattering and analyzer acceptance [2,3]. This measurement simulation routine is based on a Monte-Carlo simulation of electron paths in a small surface volume, which can be filled in principle with any element distribution. (II) Demonstration of a modified common straight-line approximation based EXCEL-routine for ARXPS data evaluation, which applies a simple empiric angle correction in the high-angle region [4]. The two correction parameters, i.e. angle and strength, have to be determined from a known thin film standard and can later on be implemented for similar unknown structures. (III) Examples for multiple well-approximated solutions found for simulated ARXPS measurements at exactly-defined but more complex surface structures. Here the necessity of the use of problem-specific boundary conditions is underlined.

As a summary it is concluded that measurement simulation is a very useful tool for the estimation of the limits of ARXPS interpretation and that the careful use of high-angle information can be helpful in the case of special surface structures. Nevertheless the lack of information content cannot be overcome.

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Utilizing Artificial Neural Networks for the Automation of Auger Spectra Analysis

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The use of Artificial Neural Networks (ANN) is a quick and efficient way for analyzing data for different purposes. Apart from realizing relationships within a set of measured data, ANN may be also trained with a set of data containing specific features, and then look for a match of the learned feature in a new set of data.

These properties of ANN are very useful in our research work when we have in mind that the main goal of our work is the full automation of the Auger spectra analysis. The relationship realization capability of the ANN was used to "deconstruct" the standard Auger spectrum of various elements into its parts as a necessary step to build the Auger spectra simulator which would later be used to test algorithms for background removal and noise reduction. The fact that we were not looking for the justification on the physical basis but were taking into consideration features as they were needs to be emphasized here, and ANN are capable of predicting relationships in a given data without knowing the details of the physical phenomena behind it, i.e. without presenting an equation to the program. Having the pattern matching capability on the other hand yet unexplored in this context we think that ANN can be utilized in a variety of ways to analyze the Auger spectra, and through this contribution we aim to shed more light into the strengths and weaknesses of using such an approach for the aforementioned purpose.

Plasmon-enhanced secondary electron emission from copper phthalocyanine deposited on Al(111)

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Aluminum \copper phthalocyanine (CuPC) interface is relevant in applications such as organic solar cells consisting of Al\CuPC\Ag thin layers that have shown enhancement of photoelectron conversion efficiency by surface plasmon excitation [1] . Furthermore, STM induced light emission from metal phthalocianine films on metal surfaces have been observed to enhance via plasmon excitation in the metal substrate [2]. In this paper coupling of the metal substrate plasmon excitation with the CuPC ionization is studied through observation of the secondary electron yield. Early experiments on Al(100) [3,4] propose that secondary electrons are emitted via a mechanism similar to photoemission with plasmon decay playing the role of photon absorption. The system studied is a 4Å thick CuPC film deposited in vacuum on Al(111) surface. The Al bulk plasmon is excited by electron impact in specular reflection geometry and the secondary electron spectrum is acquired in coincidence. The secondary electron spectrum coincident with the bulk plasmon excitation is fully interpreted in terms of photoemission events from CuPC initiated by pseudo-photons with energy equal to the bulk plasmon electron energy loss. These findings suggest that the plasmon de-excitation generates an intense electromagnetic field at the interface that is responsible for the molecular ionization.

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ARXPS on Surface Pre-Treatments for $LiNbO_3$ SAW substrate

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The analysis of surfaces/interfaces and thin films is vital for the improvement of surface acoustic wave (SAW) devices. Such modern devices are characterised by the trend to higher frequencies, power densities and new applications. Therefore, a shrinking of the dimensions is necessary but hardly possible to achieve with standard Al based metallisation due to increased stress-induced damaging (acoustomigration). Better results can be obtained by highly textured metallisations which were recently developed [1,2]. In this context an additional barrier interlayer is necessary and a pre-treatment of the substrate. Furthermore, a Variation of the deposition parameters ar an additional heat treatment might be of great interest.

This work gives an overview about studies of the effect of surface preparation at $LiNbO_3$ for a Ta deposition used as barrier material. A radio-frequent plasma and a focused ion beam are applied for surface treatment; a dc-sputter process is used for the deposition of Ta. An e-beam evaporation system is used for the toplayer deposition (Al). The characterisation of the surface's and interfaces' chemical changes is done mainly by means of X-ray photoelectron spectroscopy (XPS) directly coupled to a preparation chamber (quasi in situ). Applying the angle-resolved XPS method (AR-XPS), in-depth information can be obtained without sputtering using an improved mathematical approach [3-5].

Funding of the work by DFG (Grant No. OS 115/8-1) is acknowledged.

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IUVSTA71 Abstracts
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Model studies of the validity of trajectory methods for calculating very low energy (< 100 eV) electron transport in condensed media

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Trajectory methods, for example conventional detailed Monte Carlo trajectory simulation, are often used to calculate plural or multiple scattering of electrons in matter. However, due to the neglect of coherent scattering they cannot be generally valid, but must be regarded as a fortunately useful approximation of quantum scattering. In particular, one may suspect that coherence effect should be more strong with a larger wavelength, causing trajectory methods to fail at low electron energies.

In order to study the limits of validity of trajectory methods, one may, if possible, compare them to a corresponding quantum calculation. Such calculations, which involve multiple wave scattering within clusters of atoms, are in general too complex to permit a comparison of scattering in, for example, amorphous matter, within reasonable computer time. There is however one case which permits a both rapid and exact quantum calculation, and that is the multiple elastic scattering of an electron in a cluster of point scatterers. It has recently been shown that this case can be extended to include a model of plural inelastic scattering.

Using this method of comparison, the object in which the electron scattering occurs is a cluster with a size of a few nm, containing about 10^3 more or less randomly distributed point scatterers, each scatterer modelling an atom. This may seem a poor model for a real scattering medium, such as bulk amorphous solid or bulk liquid. However, the point scatterer is not a physically unreasonable model at very low electron energies, and simple phase considerations suggest that the validity limits obtained with the point scatterer model should be similar to those obtained for electrons in real amorphous solids or liquids.

The presentation aims to give 1) a brief look at the theory of quantum scattering in a cluster of point scatterers, 2) the most recent procedure used for comparison with a corresponding trajectory simulation, and 3) the most important results so far.

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Inelastic collisions of charged particles: PWBA and asymptotic Bethe formulas

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The Plane-Wave Born Approximation (PWBA) is the basis of the conventional (Bethe) theory of stopping of fast charged particles [1-2]. The central results of the theory are the familiar Bethe asymptotic formulas for the ionization cross section and the stopping cross section. The Bethe theory takes its most transparent form in the case of collisions with atoms, described by means of an independent-electron model.

Numerical calculations of the generalized oscillator strengths (GOS) and double-differential cross sections for the self-consistent DHFS potential will be briefly described. We have generated a complete tabulation of GOSs for all subshells of ground-state configurations of neutral atoms of the elements ($Z = 1$ to 99) [3]. By using these GOSs, doubly-differential cross sections (DDCS), differential in the energy-loss and the scattering angle of the projectile, are readily evaluated. “Exact” (within the PWBA) total cross sections and stopping cross sections can then be obtained by numerical integration of the DDCS.

In the derivation of the Bethe formulas, only the global topological properties of the GOS and the Bethe sum rule are employed. Relativistic effects cause small deviations from the Bethe sum rule, and a slight modification in the definition of the Bethe parameters. Although the DHFS independent-electron model is not expected to be realistic for excitations of outer subshells, it does provide reliable values of the so-called shell corrections (*i.e.*, the difference between the exact PWBA cross section and the Bethe formula), which originate mostly from the “closing” of inner shells. Examples of calculated shell corrections will be presented.

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Mapping the surface structural and electronic properties of individual nanoparticles with the tiny beam of a Scanning Transmission Electron Microscope (STEM)

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Aberration-corrected scanning transmission electron microscopes deliver Angström-sized electron probes of typically 40 to 200 kV kinetic energy, on individual nanoparticles, outside of them, on the apex of one of their external surfaces or through them. They constitute very powerful tools to investigate both the structural and electronic properties of the selected targets at the finest spatial resolution. As a result of the strong interactions between probe and matter, many different signals can be picked simultaneously (see figure below). Electrons scattered at large angles are collected by annular detectors and they deliver signals which are of use for reconstructing, atom by atom, the 3D structure of individual nanocrystals. In parallel, electron energy-loss spectroscopy (EELS) records the electronic excitation spectrum of the specimen over a very broad domain, typically from 1 to 1000 eV, with a high level of spatial and energy resolution. When using the core-loss signals, single atom sensitivity has been demonstrated and elemental maps, atomic column by atomic column, of crystallized nanoparticles or across interfaces, are now routinely available. In some cases, taking benefit of the fine structures appearing on the characteristic edges, the bonding state of the atoms across nanostructures and at their surfaces is also accessible. In the 1 to 5 eV range encompassing the visible spectral domain, one maps the distribution in energy and in intensity of the surface plasmon modes at metal surfaces with a spatial resolution typically down to 1 nm and an energy resolution of 100 meV. It thus constitutes a very efficient technique to explore the sub-wavelength spatial variation of the electro-magnetic fields associated to surface plasmons. This is therefore a powerful alternative to near-field optical microscopy, with much increased spatial resolution, for investigating a broad range of photonic modes in very diversified geometries. Quite recently, spectrum-imaging of the emitted photons under the primary electron beam and the spectacular introduction of time-resolved techniques down to the fs-time domain, have constituted innovative keys for the development and use of a brand new multi-dimensional and multi-signal electron microscopy.

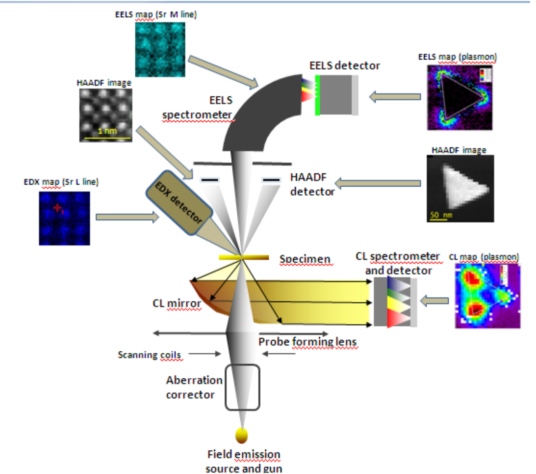

Illustration of the multi-signal strategy in a modern STEM instrument, displaying two channels of parallel information : ADF, EELS and EDX elemental mapping of the atomic structure and composition in $SrTiO_3$ (left) ; ADF, EELS plasmon map and cathode-luminescence (CL = photon emission spectroscopy) on a single Ag nanoplatelet (right)

Near and Far-Field Spectroscopy at the Nanoscale using Focused Electron Beams

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Abstract

The fascinating world of nanoplasmonics is explored here by means of focused e-beams. Thin gold films patterned with sub-micrometer holes are known for their unusual optical properties and extraordinary optical transmission (EOT) in particular. Using electron energy loss spectroscopy (EELS) in scanning transmission electron microscopy (STEM), we carefully scan the electric fields within the holes to study the crossover between near-filed and far-field regimes. The e-beam coupling to radiative modes is not trivial, yet it offers unique advantages as a probe of *optical* phenomena. Series of cavity standing waves are thus resolved, with selective appearance near specific hole faces. Moreover, intriguing details from the very early, femtosecond-scale stages of signal propagation from one hole to its neighbor are revealed, obeing particularly high *inter*slit interactions, about an order of magnitude larger than the *intra*slit edge to edge coupling. Pronounced signal enhancements and line narrowing that characterize the interslit interactions are further quantified and used to shed light on the mechanisms giving rise to efficient EOT.

Practical XPS Analysis of Nanoparticles

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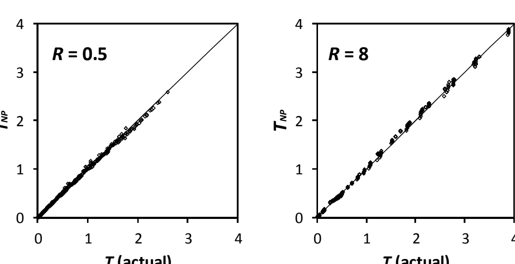
Detailed characterisation and measurement of nanoparticles is of vital importance in understanding their function and behavior. There is major interest in the application of engineered nanomaterials to enhance performance, with applications in diverse areas such as cosmetics, fabrics, catalysts, medical and electronic devices. Concurrently, there is public concern over the potential dangers that such materials pose to human health and the environment. In all these areas, the ability to measure important parameters, such as shape, agglomeration state, size and chemistry in a representative and accurate manner is vital. In many applications, the chemistry of the particle surface, or shell, defines the properties of the material in terms of processing behavior, distribution and agglomeration and functional performance. It is therefore no surprise that surface chemical analytical techniques, such as XPS should be applied to nanomaterials to determine the surface chemistry. This talk will describe the application of XPS and other techniques to nanoparticles of biological and biomedical relevance, covering the practical issues of sample preparation and the interpretation of data. The interpretation of data is of particular importance, since it should be recognised that most analysts do not have the time or expertise for detailed simulations. Therefore simple approaches and algorithms that do not significantly compromise the accuracy of the result are required [1,2]. A simple method for determining the shell thickness for spherical core-shell nanoparticles, demonstrated in Figure 1, will also be presented [3].



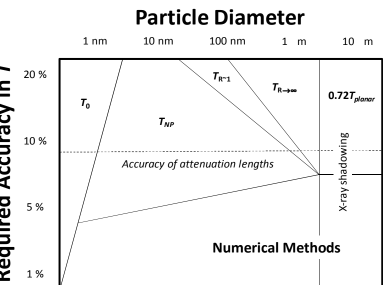


Figure 1. Left, results from a direct equation to estimate shell thickness (T_{NP}) with different particle core radii. Right, guide to the use of various equations for shell thickness on particles.

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Traceable Thickness Measurement of nm Oxide Films by XPS

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The continual scaling down of semiconductor devices means that advanced semiconductor devices require gate dielectric materials with a thickness of less than 1 nm. Oxide materials have a high dielectric constant; HfO_2, for example, is one of the most promising dielectric materials that can be used as an alternative to SiO_2. To date, however, no physical or chemical methods have been able to accurately measure the thickness of ultrathin oxides.

X-ray photoelectron spectroscopy (XPS) is ideal for measuring the thickness of ultrathin oxide film because, as a chemical method, it determines the thickness from the amount of chemicals in the oxide film. XPS has also been used to measure subnanometer SiO_2 films. However, for the thickness measurement by XPS, the effective attenuation length (EAL) of photoelectrons should be precisely determined at the given experimental conditions because it is a variable depending on the specified geometry of the spectrometer and the setting parameters due to the effects of elastic scattering.

Thickness measurement of nanoscale SiO_2 films on Si(100) substrates was the first subject of an international study conducted by surface analysis working group of the consultative committee for amount of substance from a pilot study P-38 and a key comparison K-32. In this presentation, a traceable method to determine the thickness of the ultrathin oxide films will be introduced and some results on the thickness measurement of oxide films will be discussed. Additionally, some issues for the precise thickness measurement of oxide films by XPS will be discussed.

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Sample-Morphology Effects on XPS Peak Intensities: Estimation of Detection Limits for Buried Thin Films

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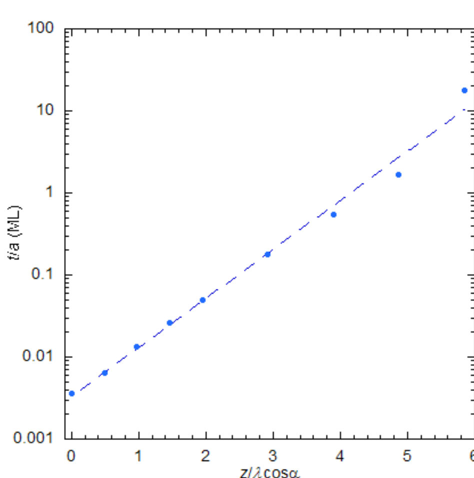
It has long been known that variations in sample morphology can have drastic effects on photoelectron intensities in XPS and thus on the results of quantitative analyses [1]. While detection limits for minor species in homogeneous samples have often been estimated to be between 0.1 and 1 atomic percent, no estimates are generally available for inhomogeneous samples. In general, detection limits depend on the detectability of a particular peak (which depends on the peak-detection method, the measurement statistics, peak identification, and interpretation in relation to the known or assumed sample morphology).

We have used the NIST Database for the Simulation of Electron Spectra for Surface Analysis (SESSA) [2,3] to estimate detection limits for buried thin films. Test simulations have been performed for thin W films of varying thicknesses buried at varying depths in a Ru matrix. For these simulations, the X-rays were incident normally on the sample and the photoelectrons were detected at an emission angle, α, of 55° with respect to the sample normal. We initially established that the W $4d_{5/2}$ peak intensity would likely be detectable in a $RuW_{0.001}$ alloy (for which the ratio of the W $4d_{5/2}$ peak intensity to the Ru $3d_{5/2}$ peak intensity was 1.25×10^{-3}). Simulations were then performed with a thin W film on a Ru substrate and for thin W films at selected depths in the Ru matrix. In each case, we varied the W film thickness, t, to obtain the same W $4d_{5/2}$ peak intensity (within 1%) as for the $RuW_{0.001}$ alloy. The Figure shows the ratio of t to the average atomic size, a, to give the relative film thickness in monolayers (MLs) as a function of the ratio of the film depth, z, to the inelastic mean free path, λ_i, of W $4d_{5/2}$ photoelectrons in the Ru matrix. We see that the defined detection limit in this example varies by over three orders of magnitude for a thin W surface film to a W film buried to depths up to $6\lambda_i$.



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Experimental Effective Attenuation Length for applications in Hard X-ray photoelectron spectroscopy

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Nowadays, the great challenge in materials science is the incorporation of complex systems in the area of the nano-technologies. Material composites, which combine different materials mostly multilayer thin films, with specific and defined properties, are a promising way to create products with specific properties. The photoemission and the Auger electron spectroscopies play a preponderant role in the study of the electronic properties of matter. Third generation synchrotron radiation sources enables the extension of XPS to higher electron kinetic energies (HAXPES, Hard X-ray PhotoElectron Spectroscopy) compensating the decrease of the photoionization cross-section for excitation energies in the hard X-ray region. HAXPES allows the accessibility to buried interfaces and bulk materials due to the dramatic increase of the effective attenuation length (EAL). Electronic, compositional and chemical depth profiles can be then performed in a non-destructive way over the tens-of nanometers scale with nanometer depth resolution. Such an important application of HAXPES is crucial for many condensed matter experiments and requires reliable EALs for high kinetic energy. EALs are well established for electrons with kinetic energies up to 2 keV. Even if EALs can be obtained by extrapolating well-known formulae, there is a lack of experimental data in the energy range between 1 and 15 keV, necessary to validate (or not) the proposed formulae. In the present study we have determined the EAL dependency on kinetic energy for titanium nitride (TiN), hafnium oxide (HfO_2), silicon (Si), silicon dioxide (SiO_2), lanthanum lutetium oxide ($LaLuO_3$), lanthanum calcium manganite ($La_{0.66}Ca_{0.33}MnO_3$), and gold (Au) from 1 keV up to 15 keV. A correlation between the EAL energy dependence and the material density is established. The EALs has been obtained by following either core level peak intensity dependence for a fixed kinetic energy as a function of the overlayer thickness or the core level peak intensity dependence with the photoelectron kinetic energy (i.e. photon energy) for a fixed overlayer thickness. The experimental set-up used is devoted to the combination of X-ray Diffraction (XRD) and HAXPES. Hence, we are able to determine the exact thickness and roughness of the layer from a fit of the X-ray reflectivity (Kiessig fringes) and simultaneously to obtain the EALs from the HAXPES signal evolution. It is important to stress that due to the simultaneous detection of the diffracted and photoemitted signal, the EALs, thickness and roughness determination correspond exactly to the same sample region.

IUVSTA71 Abstracts
Thursday, June 27

PROBING THE COMPOSITION, ELECTRONIC AND MAGNETIC PROPERTIES OF BULK MATERIALS, BURIED LAYERS AND INTERFACES WITH STANDING-WAVE AND HARD-X-RAY PHOTOEMISSION

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I will present some new directions in soft x-ray photoemission (XPS, SXPS) and hard x-ray photoemission (HXPS, HAXPES, HIKE) [1-16]. These involve combined SXPS and HXPS studies of buried layers and interfaces in magnetic and transition-metal oxide multilayers [5,6,8,10,12], hard x-ray photoemission studies of the bulk electronic structure of some spintronic materials [4,7,11,14]; band-offset measurements in oxide multilayers[12]; the use of standing waves from multilayer mirrors to enhance depth contrast in spectroscopy [1,5,6,10,15,16], as well as in angle-resolved photoemission (ARPES) [1,5] and photoelectron microscopy [3]; and the prospects for carrying out bulk sensitive hard x-ray ARPES (HARPES) [9,14,16] and hard x-ray photoelectron diffraction (HXPD) [2].

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Electronic characterization of nano-structured materials by HAXPES

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Photoelectron spectroscopy (PES) is a well-established and effective tool for electronic structure investigation at solid surfaces. The inherent high surface sensitivity of conventional PES is overcome by using hard X-ray excitation in the multi keV range (HAXPES), where energetic photoelectrons emerge from deeper inside the material due to their significantly increased inelastic mean free paths. It then becomes possible to also study electronic properties of complex bulk materials and/or at buried interfaces.

Because photoelectric cross sections rapidly decrease with photon energy above ionization thresholds, the use of brilliant and tunable undulator radiation at 3rd generation synchrotron sources is greatly enhancing the effectiveness of this technique which is rapidly emerging at storage ring facilities worldwide. X-rays in the range 3 to 12 keV are typically used allowing to probe electronic and chemical structure down to a depth of about 10-20 nm.

This bulk sensitivity not only is essential in the study of complex correlated materials, which often exhibit a modified surface electronic structure, but also indispensable for technologically relevant multi-layered materials with buried interfaces. Most interesting for materials science applications is the ability to study *as-grown* materials without any need for prior *in-situ* surface treatment or sensitive structures covered by protective metallic layers. Since recently, e.g. *functional* materials such as MIM-structures showing resistive switching behavior are being studied by HAXPES under "*in-operando*" conditions. An overview will be given on the current state of the technique at the PETRA III facility and other instruments worldwide, highlighting its great potential by recent scientific results.

Intrinsic and surface excitations in XPS/HAXPES

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In addition to effects of electron transport - in an infinite solid - on the spectra of electrons induced by photons, intrinsic excitations due to the sudden appearance of atomic core holes and surface excitations due to the presence of the solid-vacuum interface can influence the observable electron spectra considerably. Therefore the deeper understanding of such intrinsic and surface excitation phenomena taking place in solid systems is necessary for the accurate surface and interface chemical analysis.

Intrinsic excitations localized to the close environment of the atom with the core hole can result in shakeup satellite structures in the energy loss part of the photoelectron or Auger peaks, the creation of electron-hole pairs in conduction bands of metals can lead to peak asymmetry and excitation of plasmons by the suddenly created core holes can yield plasmon loss satellite structures in the spectra.

The surface/interface crossings of the electrons are accompanied by surface/interface excitations leading to surface/interface plasmon loss satellites of the photoelectron or Auger peaks.

Methods for describing the photon energy dependence of the intensity of shakeup satellite peaks and their energy separation from the main photoelectron or Auger peaks, as well as the asymmetry of these main peaks are discussed in comparison with recent experimental results obtained for 3d transition metals. Approaches for describing effects of intrinsic plasmon excitations on photon induced electron spectra of metals and semiconductors, including interference phenomena between intrinsic and extrinsic plasmon excitations, are discussed demonstrating the role and photon energy dependence of these effects. Problems of separating effects of intrinsic and extrinsic plasmon excitations, especially in the case of nanostructures and low photon energies are detailed. Effects of surface plasmon excitations, their dependence on electron energy and emission angle, methods for modeling surface excitations (including the approach describing the combined effects due to the surface and core hole) and deriving electron transport parameters from experiments to characterize effects of surface excitations on photon induced electron spectra, are summarized.

Quantification of XPS Analysis of Stratified Samples

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An analysis of inhomogeneous samples with a complicated morphology is a frequent application of X-ray photoelectron spectroscopy. The stratified samples, with uniform lateral compositions of layers parallel to the surface, are the idealized examples of inhomogeneities. Devices with surface region consisting of planar structures of different materials exhibit properties that are of current technological interest.

Theoretical models describing the photoelectron transport in multilayer samples are compared and discussed. These models are applied to different multilayer systems with layers of varying thicknesses. An extension of the definition of the emission depth distribution function (EMDDF) is discussed, and exemplary calculations of this function are shown. The EMDDF for a layer deposited at a surface turns out to be identical as for the bulk of the layer material, however it may differ considerably when the layer is buried at a certain depth [1]. The EMDDFs for buried layers are found to be considerably affected by elastic photoelectron scattering, however in a different way as the EMDDF for the bulk material. The XPS depth profiles calculated for multilayer materials are noticeably affected by elastic photoelectron collisions.

Photoelectron signal intensities calculated for a thin overlayer on a uniform substrate from theoretical models taking elastic photoelectron collisions into account are shown to be very weakly dependent on the substrate material. This result has been obtained for photoelectrons analyzed in XPS spectrometers equipped with typical X-ray sources, i.e. sources of Mg Kα and Al Kα radiation. Consequently, an analytical model that can accurately describe the photoelectron intensity from an overlayer deposited on any material (e.g. on a substrate of the same material as the overlayer) can be a useful basis for a universal and convenient method for determination of the overlayer thickness [2]. An example of such analytical formalism based on the dipole approximation is discussed. It is also shown that the postulated method for overlayer-thickness measurements does not need time-consuming Monte Carlo simulations of photoelectron transport, and does not require knowledge of the effective attenuation lengths. Unfortunately, due to small information depth, this method is applicable to layers of small thicknesses. This limitation can be circumvented by the use of high-energy photoelectrons. An extension of formalism to Zr Lα and Ti Kα radiation sources, involving the multipole photoemission cross section, is briefly discussed.

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Energy loss functions and IMFPs derived by factor analysis of reflection electron energy loss spectra

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The energy loss function (ELF) given by optical constant is the basis of the fields of the estimation of inelastic mean free path (IMFP) and background spectra for the quantitative surface chemical analysis by electron spectroscopies. The optical constants are evaluated by optical measurements of reflectivity/absorption coefficients and have been collected into handbooks and databases. But in high energy vacuum-ultraviolet (VUV) region, optical experimental data are often missing because this requires synchrotron radiation photon sources. Another approach to evaluate the ELFs is the analysis of electron energy loss spectra (EELS), which can be easily measured in the VUV energy region with a standard laboratory electron spectrometer. However, EELS spectra include complicated factors: surface energy loss, multiple inelastic scattering, interference effects, momentum transfer and so on. Especially, the contribution of the surface energy loss is inevitable for the reflection-type EELS (REELS) measurement. For determining ELFs and optical constants, one has to extract the bulk energy-loss-structures from the REELS spectra by subtracting the contribution of the surface energy-loss. Many previous works have been done for determining ELFs from REELS measurements. They require stoichiometric clean surfaces to which theoretical formula linking a relation between bulk and surface energy-loss-structures are applicable. It was not easy to determine the ELFs of chemical compounds that easily become non-stoichiometric by surface ion-beam cleaning. Therefore, stoichiometric clean surface is a tough prerequisite for previous methods.

In order to avoid the tough prerequisite for the analysis of chemical compounds, we successfully obtained the bulk ELFs for semiconductors by applying the factor analysis method to a series of primary-energy-dependent and emission-angle-dependent REELS spectra. This factor analysis method is based on a multivariate analysis of REELS spectra and does not require a delicate theoretical evaluation of the surface energy-loss-structure. Moreover, we have demonstrated that this method is useful to evaluate bulk ELFs and optical constants for compound semiconductive-materials (GaAs, GaSb etc.) with damaged surface-layer or contaminated surface whose surface energy-loss-structures can not be evaluated theoretically. It means that this practical method does not require ideally-clean surfaces and eases the prerequisite for various compound materials.

PHOIBOS 225 HV: High energy electron spectrometers with wide acceptance angle pre-lens

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The PHOIBOS 225 HV is a hemispherical electron analyzer with unsurpassed transmission, energy and angular resolution. The multi-element transfer lens is optimized for ultimate energy resolution up to highest kinetic energies and can be operated in several different modes for angular or spatially resolved studies. The modular power supply concept makes it suitable for every aspect of electron spectroscopy: from laser based ARPES measurements at low kinetic energies starting at virtually zero kinetic energy, to quantitative XPS and high energy photoemission spectroscopy at electron energies of up to 15 keV. An additional pre-lens extends the acceptance angle to up to +/- 30°. This increases the transmission of the analyzer and enables angular resolved XPS for non-destructive depth profiling without any sample rotation.

Several detector options with high sensitivity and dynamic range are available: 2D-CCD detector with a Peltier cooled camera, 1D and 2D-delayline detectors, and combined 2D-CCD(DLD)/SPIN detectors. Especially the DLD detectors are ideally suited for data acquisition under extreme conditions as they occur in HAXPES experiments. Here, the DLD detectors with their improved sensitivity, lateral and time resolution allow the detection of spectroscopic features with a count rates 5 counts/second or less can be detected.

Electron beam induced changes in Auger electron spectra for Lithium ion battery materials

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The so called solid electrolyte interphase (SEI) [1], a thin film on top of the electrodes of common lithium ion batteries has an important role for the lifetime and the performance of such cells. Due to its surface and chemical sensitivity the state of the art tool for investigations of this layer is the X-ray photoelectron spectroscopy (XPS). Since the SEI can consist of several different organic and inorganic compounds with a size down to some nm [2], a technique with the same surface and almost the same chemical sensitivity but a high spatial resolution would be very desirable. In this work we try to apply Auger electron spectroscopy (AES) to this field of lithium based materials.

The different excitation by electrons in AES in contrast to X-rays in XPS leads to several problems for the detection of lithium compounds in the SEI. Most of the SEI components are not conductive, so the effects of charging are commonly the biggest ones. In addition the electron beam can cause a change and a damage of the sample surface [3]. In this work we performed a lot of reference experiments measuring pure lithium, lithium compounds and reaction products of lithium with common electrolyte ingredients, regarding their stability and their distinctness in AES analysis.

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Electron scattering in graphene/copper system

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Electron scattering at solid surfaces has been of crucial importance for electron spectroscopy methods. With the growth of nanotechnology, the interest in the details of the dynamics of electrons near a vacuum-solid or solid-solid boundary has seen a remarkable revival. The electron inelastic and elastic scattering is well understood for bulk solids. For new class of two-dimensional materials (2DM) such as graphene and silicene on substrates, electron scattering mechanism is not fully understood and, thus, electron spectroscopy data could not be properly interpreted. In this contribution, graphene is grown on polycrystalline copper substrates by CVD method [1]. This system will be measured by X-ray induced angular resolved photoelectron spectroscopy and by reflection electron energy loss spectroscopy. Obtained data will be compared with the state-of-the-art theoretical approaches. On the basis of the comparison the validity or invalidity of available theoretical models developed for bulk solids or thick overlayers and applied to the 2DM film/substrate systems will be discussed.

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Surface characterization of ZnO and Ag loaded metal oxide nanotubes using spectroscopic techniques

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Synthesis and formation of nanoscale oxide layers on metallic surfaces has recently drawn much attention in many fields of materials research. To date, a large part of the interest has remained on titanium oxide (TiO_2) nanotubes using electrochemical anodization process. A similar self-assembled mechanism as for TiO_2 nanotubes leads to the formation of zirconium oxide (ZrO_2) nanotubes, which may also be a promising substrate for various applications, especially in biomedicine.

In this work we have fabricated nanoporous oxide layers on Ti and Zr with the addition of Ag or ZnO nanoparticles in order to obtain medical coatings ensuring both biocompatibility and antibacterial properties. The fabrication strategies of TiO_2 and ZrO_2 nanotubes allowed for precise control the nanotube length and diameter, thus enabled to load different amounts of nanoparticles and control the antibacterial activity. In order to reveal the morphological and chemical features, the composite coating fabricated were studied with the aid of high-resolution scanning electron microscopy (SEM) combined with energy dispersive X-ray spectroscopy (EDX) and surface analytical techniques: AES, XPS.

Our results have shown that Ag nanoparticles can be incorporated in a simple and economic manner, suitable for the fabrication of new types of bactericidal materials The nanoparticles are distributed homogeneously in the coating, which is promising to for maintaining a steady antibacterial effect. The Ag appears in the composite layers mostly as metal silver. The amount of the nanoparticles is variable and depends on the deposition process conditions.

Acknowledgements

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Combined nano-AES and EDS characterization of materials

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In recent years, Auger spectroscopy has been neglected on benefit of X-Ray photoelectron spectroscopy giving an easier access to the surface composition and chemical shift. Indeed, thanks to new generation electron sources, developed for high resolution microscopy, ultimate probe size of 10 nm is achieved with the new generation Auger nano-probes. Such equipments are therefore promising tools to address the need of localized chemical characterization of cutting edge structures whose dimensions are reaching the nanometric scale on which "classical" XPS (X-Ray source), with spot size of 400 to 30 microns, only permits to obtain global information. In addition, with energy resolution of 0.1 % (at 2000 eV), nano-Auger electron spectroscopy is not only able to give information about the composition but also, when the chemical shift is high enough, on the chemical environment.

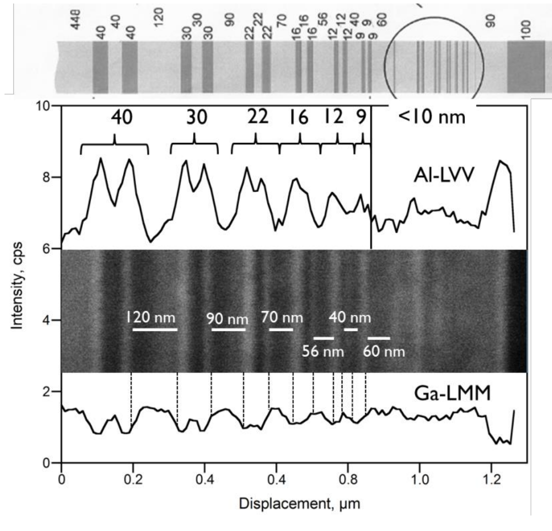

Figure 1. Al-LVV et Ga-LMM Auger line profiles and SEM image of the corresponding analysis area on a certified BAM-L200 reference sample (30 kV, 10 nA). The Al0.7Ga0.3As/GaAs stack is presented on top.

The present work is dedicated to the determination of ultimate performances of nano-Auger spectroscopy. The lateral resolution, sensitivity, topology impact are evaluated on a certified reference sample, BAM-L200 (« Bundesanstalt für Materialforschung und prüfung »), constituted of a stack of alternated lines of Al0.7Ga0.3As/GaAs with variable intervals ranging from 700 to 7 nm (Figure 1). The complementarity between AES surface measurements and EDS "bulk" analyses will be illustrated on explicit samples.

Monte Carlo simulations of low energy electron in nanostructures

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A comprehensive Monte Carlo code (MC) has been developed to explore electron-nanostructure interactions. We have adopted event by event MC simulations. The code uses accurate elastic and inelastic cross sections and includes the secondary electron generation and cascade. A nanotextured surface and a spherical nanoparticle, representing a low and a high Z number, are considered as basic geometries. KeV electron range, chosen as a probe in surface science techniques, is used in the present study to model the production of the secondary yield of electrons (SE) and the backscatterd fraction (BSE) of the primary electrons. As a central result, we show that the SE and BSE signals vary considerably with the size of the nanostructure geometry. These variations will be discussed, for the first time in the present study, in terms of collision number and energy deposited.

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IUVSTA71 Abstracts
Friday, June 28

Characterizing Nanoparticles for Environmental and Biological Applications

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For the past decade we have been studying the behaviors of nanoparticles in environmental and biological systems. This presentation will summarize some of the frequent characterization challenges inherently associated with understanding nanomaterials in these environments and provide examples of how surface and other characterization methods have helped us address some of the challenges. There is increasing recognition that published reports on the properties and behaviors of nanomaterials have often involved inadequate characterization [1]. Consequently, the value of the data in many reports is, at best, uncertain. It is necessary for researchers to recognize the challenges associated with reproducible materials synthesis, maintaining desired materials properties during handling and processing, and the dynamic nature of nanomaterials at all stages of nanoparticle preparation, characterization and use [2]. Researchers also need to understand how characterization approaches (surface and otherwise) can be used to minimize synthesis surprises and to determine how (and how quickly) materials and properties change in different environments. Some of the needs and lessons we have learned examining the ability of iron metal-core oxide-shell nanoparticle to reduce environmental contaminants [3], observing the nature of ceria nanoparticles during synthesis and aging [4] as well as how they interact with biological systems and measuring the stability of silver nanoparticles in biological media will highlight both general analysis difficulties and the value of surface sensitive analysis methods in combination with other techniques [5]. Because nanoparticles are often synthesized, supplied or used in liquid media procedures to extract particles from the media maintaining as much of the desired information as possible is important to enable analysis from surface sensitive methods such as XPS to be valuable [3]. Equally important is the application of surface sensitive methods (such as sum frequency generation) that can characterize particle surface in solution [2].

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Nanoparticles in Biomedical Applications: Characterization Challenges, Opportunities and Recent Advances

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Nanoparticles exhibit unique surface properties and require well-controlled surface properties to achieve optimum performance in complex biological or physiological fluids. Thus, there is a need to develop rigorous and detailed surface analysis methods for their characterization. The surface chemistries of oligo(ethylene glycol) (OEG) self-assembled monolayers (SAMs) on Au nanoparticle (AuNP) surfaces were characterized with x-ray photoelectron spectroscopy (XPS), time-of-flight secondary ion mass spectrometry (ToF-SIMS), Fourier transform IR spectroscopy and high-sensitivity, low-energy ion scattering (HS-LEIS). The size, shape, and size distribution of the AuNPs was determined by transmission electron microscopy (TEM).

Both methoxy (CH_3O-) and hydroxyl (HO-) terminated OEG SAMs with chains containing 11 methylene and 4 ethylene glycol units were examined. ToF-SIMS clearly differentiates the two OEG SAMs based on the $C_3H_7O^+$ peak attributed to the CH_3 terminated SAM, while XPS didn't detect a significant difference between the two SAMs on the same surface. However, XPS did show a significant difference between the same SAM on different sized AuNPs. Both OEG SAMs were more densely packed on the 40 nm diameter AuNPs compared to the 14 nm diameter AuNPs. FTIR experiments indicates the methylene backbone groups are well-ordered on all gold surfaces, but the OEG groups are more ordered on the 40 nm diameter AuNPs. Together the XPS and FTIR results suggest the OEG SAMs form a thicker and/or higher density SAMs on the 40 nm AuNPs compared to the 14nm AuNPs. HS-LEIS experiments showed the OEG SAMs on the 40 nm AuNPs were significantly thicker (2.6 nm) than the OEG SAMs on the 14 nm AuNPs (2.0 nm) and the flat Au surface (1.9 nm). The 2.6 nm thickness measured on the 40 nm AuNPs is consistent with thickness expected for a well-order OEG SAM (2.7 nm). TEM showed the 40 nm AuNPs had a larger size distribution and were less spherical compared to the 14 nm AuNPs, suggesting the shape of the AuNPs can have a significant effect on the structure and thickness of the OEG SAMs.

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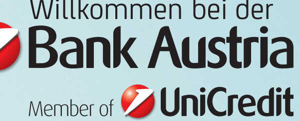

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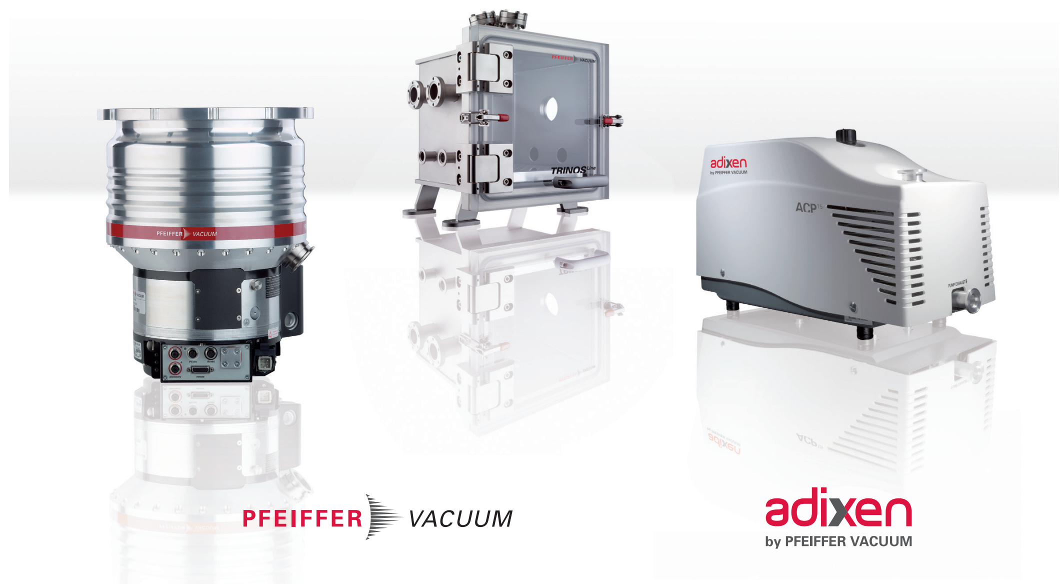

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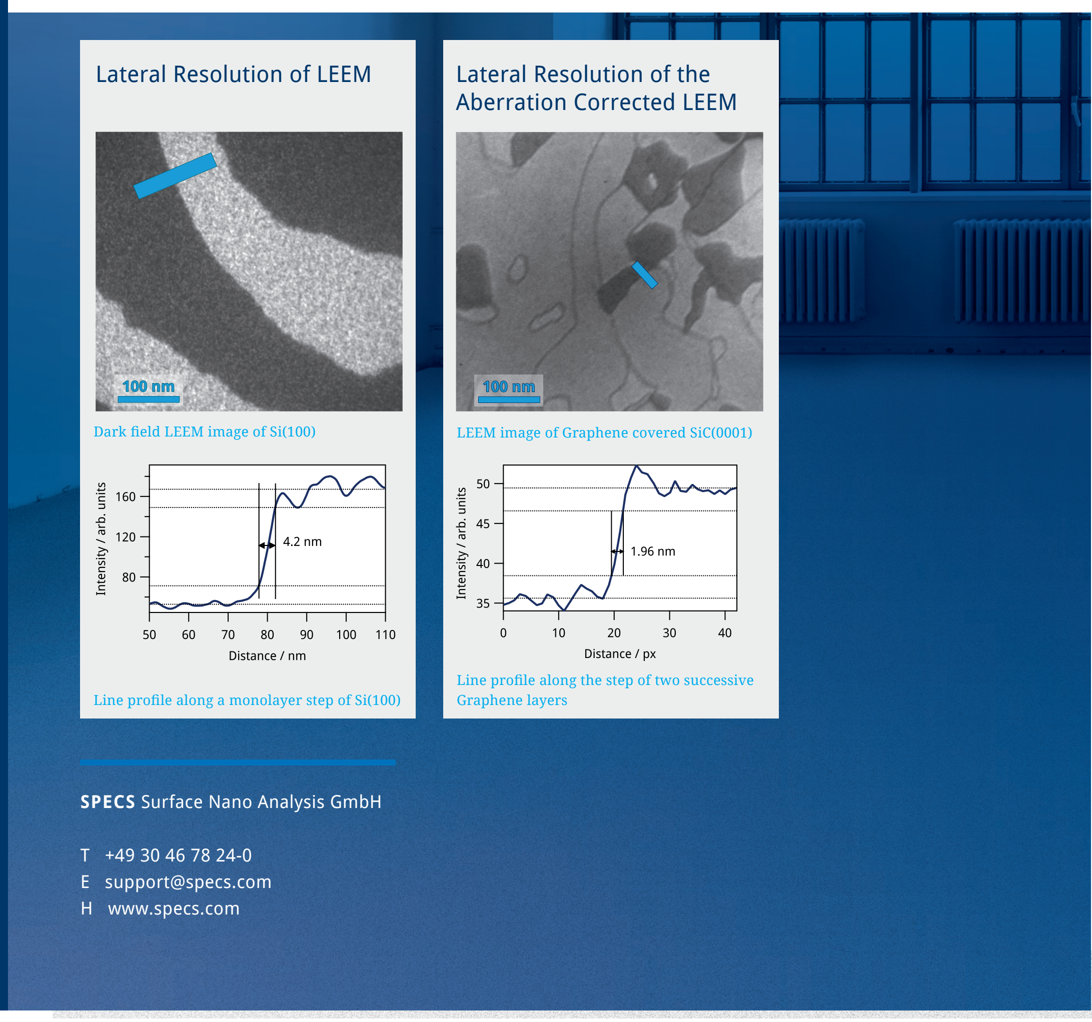

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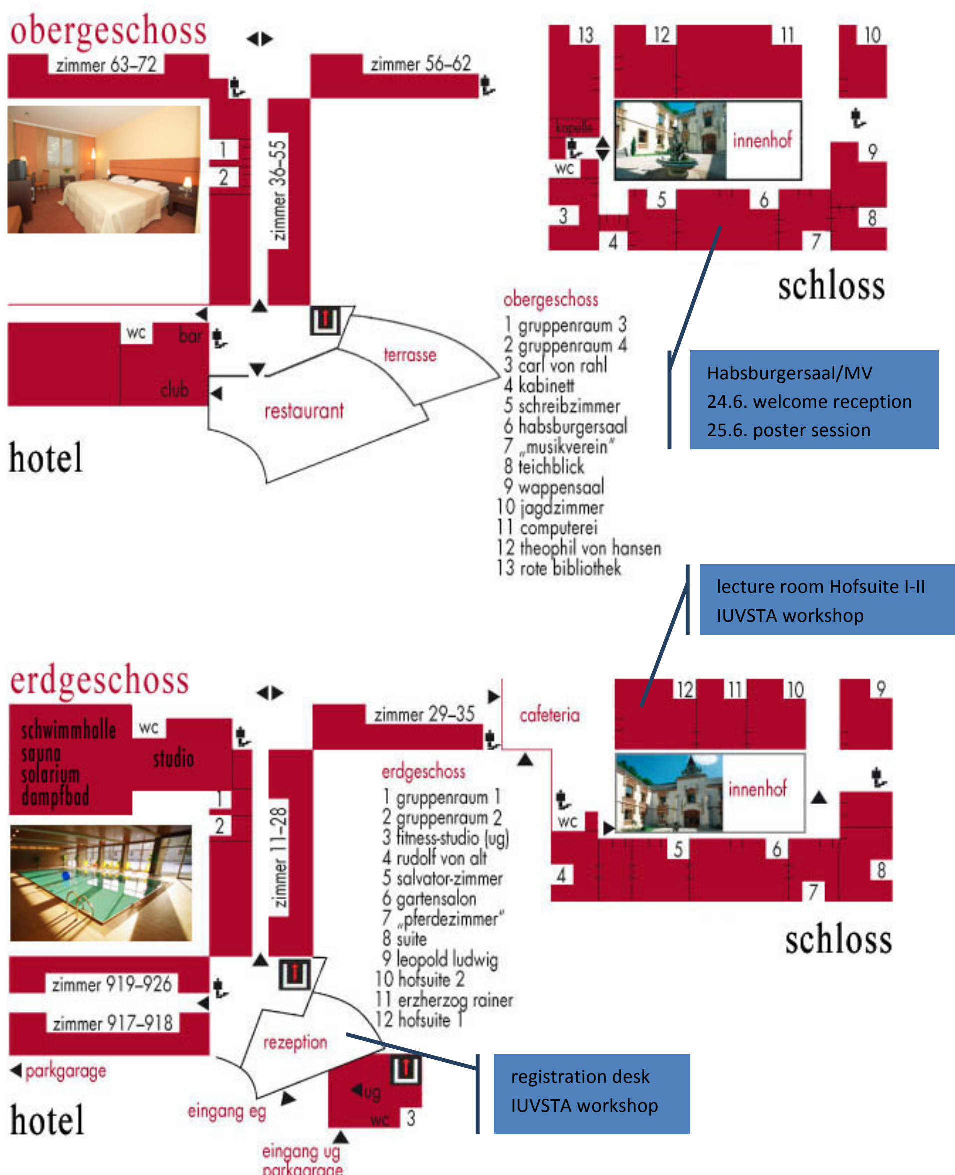

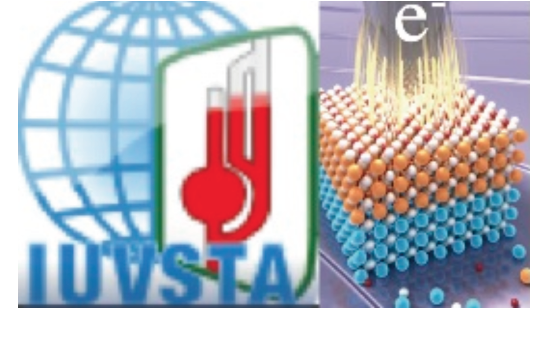

71st IUVSTA Workshop:

Characterisation of Nanostructures by means of Electron Beam Techniques

Castle Hernstein
June 24-28, 2013

Wolfgang Werner,
Cedric Powell,
Mihaly Novak

71st IUVSTA Workshop: Nanocharacterisation by Electron Beam Techniques
Programme

	Monday, june 24th	Tuesday, 25.06	Wednesday 26.06	Thursday 27.06	Friday 28.06
7:15		Breakfast			
8:30-9:00		Opening	S5: Salvat-Gavalda Liljequist	S9: Drube Fadley	S13: Baer Castner
9:00-9:30		S1: Garcia-Molina			
9:30-10:00		Tanuma			
10:00-10:30		Coffee Break			
10:30-11:00		S2: Novak Salvat-Pujol	S6: Colliex Cohen	S10: Kover Jablonski	Panel Discussion & Workshop End
11:00-11:30					
11:30-12:00					
12:00-12:30		Lunch			
12:30-13:00					
13:00-13:30					
13:30-14:00					
14:00-14:30		S3: Ding Dapor	S7: Shard Kim	S11: Yoshikawa Kampen	
14:30-15:00					
15:00-15:30					
15:30-16:00		Coffee Break			
16:00-16:30	Registration & Reception	S4: Frase Villarubia Müllerova DiFillipo Danin Winkelmann	S8: Powell Castro panel discussion	S12: Bouttemy Hoffman Jiricek Roguska Chaoui	
16:30-17:00					
17:00-17:30					
17:30-18:00		Poster Session			
18:00-19:00					
19:00-21:00	Dinner		Conference Dinner	Dinner	