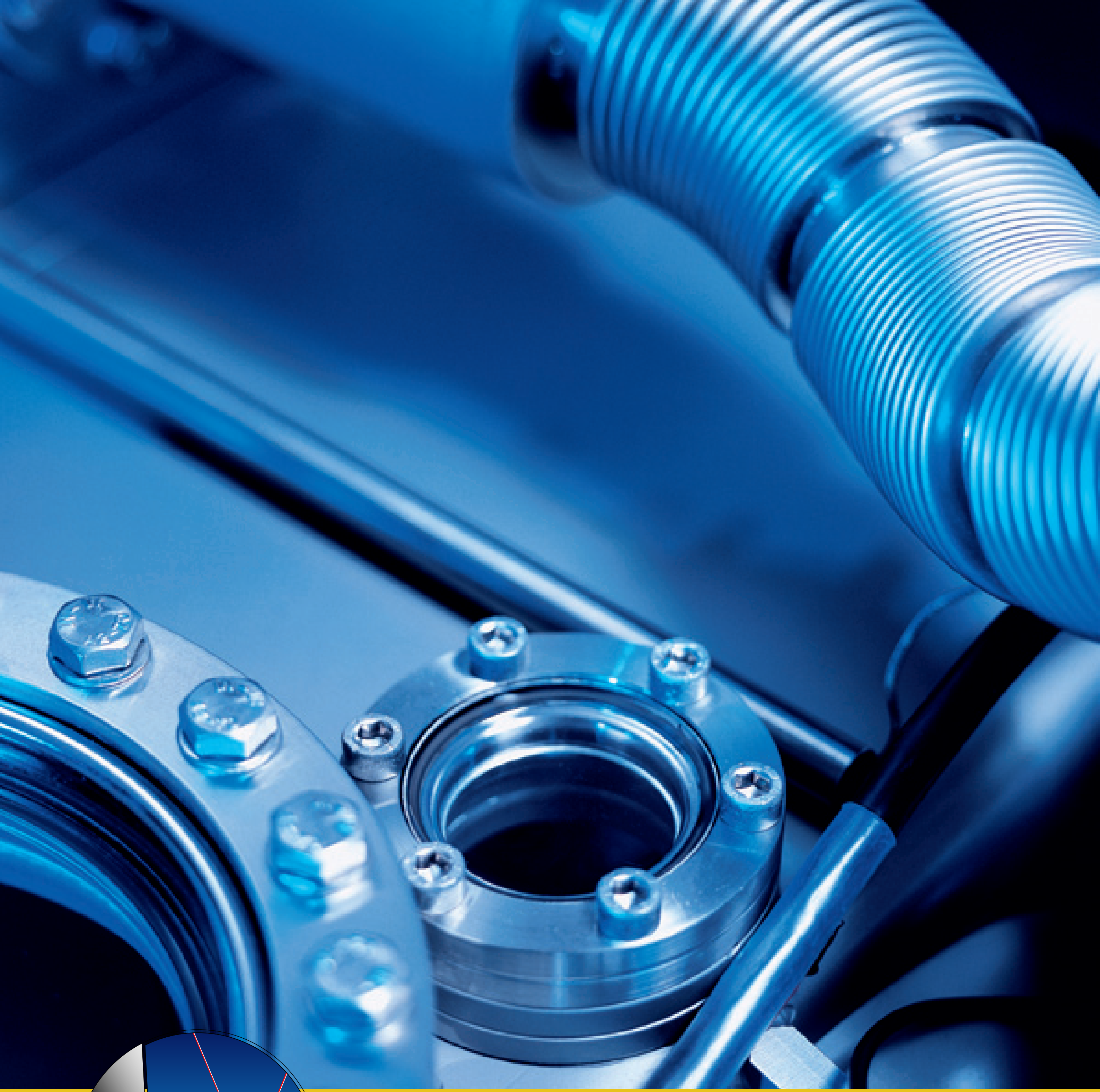


3D NanoChemiscope

Combined SIMS-SFM Instrument for the 3-Dimensional Chemical Analysis of Nanostructures

Supported by FP 7 of the European Commission

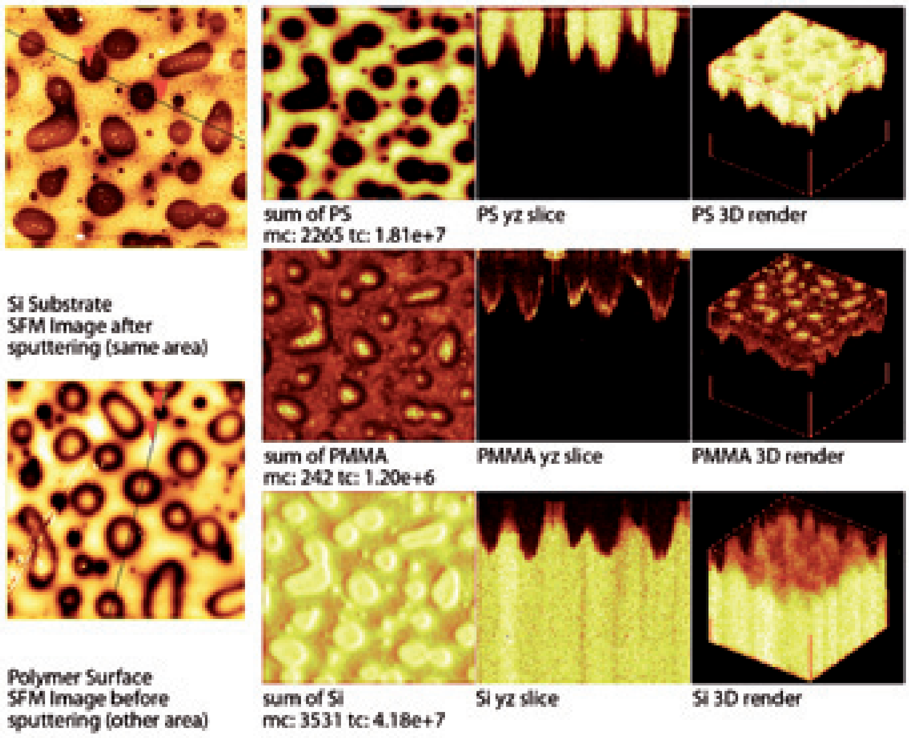
SEVENTH FRAMEWORK PROGRAMME

3D NanoChemiscope

Advances in analytical instrumentation and nanometrology have been the key to the remarkable progress in nanoscience and nanotechnology research over the last two decades. Detailed knowledge of the physical, chemical, mechanical, electronic, photonic and magnetic properties is needed in all phases of the development from exploratory research to concept and prototyping and finally manufacturing. However, the resolution, sensitivity, accuracy and analytical information provided by the existing analytical techniques are often stretched to the limits and will not at all meet the future demands of the industry.

For the analysis of ultra-thin layers and 3D nanostructures, material will be removed layer by layer in a very controlled way by using ultra low energy sputtering, cluster sputtering techniques and nano-mechanical machining with the SFM tip. The topography at the surface and at various depths will be quantitatively measured in-situ by the depth calibrated SFM. Joint by a novel software for the calculation and display of 3-dimensional distributions of all chemical species, this leads to a totally new and highly innovative „3D NanoChemiscope" with broad multidisciplinary application areas.

The scanning probe techniques and particularly Scanning Force Microscopy (SFM) in its various operation modes are widely used in nanosciences and can yield information on nanostructures with superb lateral and vertical resolution down to the atomic scale, but they lack the true chemical information which is often needed. On the other hand, all existing techniques for the chemical analysis of surfaces, interfaces and three-dimensional structures using electron, ion or photon beams have severe limitations either in lateral resolution, depth resolution or in sensitivity. An even larger gap exists for the chemical nanoanalysis of organic materials and molecular devices with high lateral resolution.



Combined AFM / TOF-SIMS study of a PMMA – PS Structure on Si

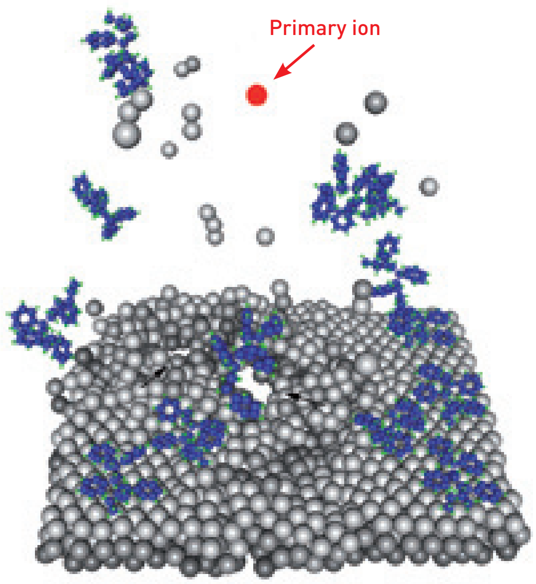
To close these gaps the consortium consisting of several well-established partners of the Network of Excellence "NanoBeams" of the FP6 programme who are leading in the field of time-of-flight secondary ion mass spectrometry (ToF-SIMS) and scientific partners with a high level of expertise in scanning force microscopy (SFM) have developed an exciting, totally new analytical concept.

The 3D NanoChemiscope NMP project started on 15th September 2008 with 8 partners from industry and public research organisations under the 7th Framework Programme of the European Commission to develop an innovative and novel combination of a new ToF-SIMS with substantially optimized lateral resolution down to at least 10 nm and improved sensitivity, combined with a new high resolution ultra-high vacuum SFM. The combination of the two techniques provides for the first time hitherto unavailable complementary information on nanoscale surface chemistry and surface morphology in one machine at the same time.

With a total budget of 4 M € and a duration of 4 years (2008-2012) this multidisciplinary project is based on the complementary know-how of the involved partners to overcome the known nanoanalytical limitations and to address problems such as molecular 3D analysis so far not solvable by any of the existing techniques. All aspects from fundamental research to applications, metrology and standardisation are well-addressed and well-balanced in this project.

TOF-SIMS

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is known to be a very versatile, extremely sensitive mass spectrometric technique that provides detailed information on the elemental as well as on the molecular composition of all kinds of solid surfaces with extremely high sensitivity.



Bombardment of a surface with energetic primary ions

The bombardment of a surface with energetic primary ions leads to the emission of atoms, clusters, intact molecules and fragments from the uppermost monolayer of a surface, and the ionised fraction of the emitted particles can be mass analysed.

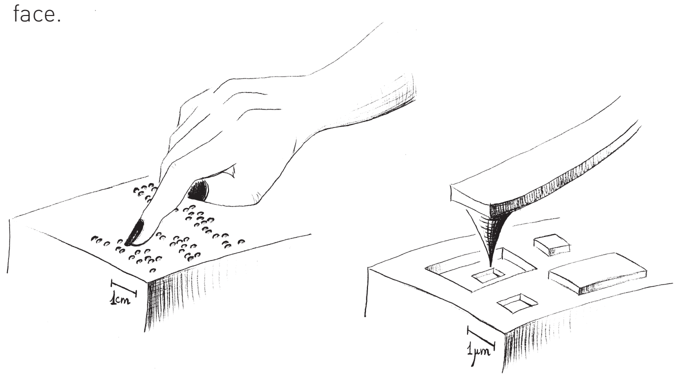
TOF mass spectrometry is a pulsed primary ion beam technique and based on the fact that secondary ions with the same energy but different masses travel with different velocities. Measuring the flight time for each ion over a fixed distance allows the determination of its mass.

The time-of-flight technique offers parallel detection of all secondary ion species with ultra-high transmission and high mass resolution. This technique can be used for virtually all kind of conductive and non-conductive materials. In the ion microprobe mode, a highly focussed ion beam is scanned over an area of interest and complete spectra are recorded for every pixel. In this way, images can be acquired for all atoms including hydrogen and molecules in parallel with high sensitivity. For a well-controlled removal of surface layers a second ion beam with low energy sputter ions like oxygen or caesium (200 eV - 2000 eV) or cluster ions is simultaneously used in order to measure depth profiles of all species with high depth resolution in the nanometer range (dual beam mode).
By the combination of imaging and sputtering, the distribution of all species in a 3-dimensional object can be analysed. For each voxel (volume pixel, 3-dimensional pixel in a 3D dataset) a complete mass spectrum with elemental and molecular information is stored. This concept enables very powerful retrospective analysis capabilities. Spectra and profiles can be reconstructed from any user-defined region of interest, images and 3D distributions for every mass of interest.
This makes the technique very powerful for the 3D analysis of complex structures with "unknown" or partially "unknown" composition.

SFM

Atomic Force Microscopy, or more generally Scanning Force Microscopy, has become the most versatile Scanning Probe Microscopy technique since its first application in 1986. Unlike the Scanning Tunneling Microscope, it is not limited to conductive surfaces: applications nowadays cover fields as varied as polymers, semi-conducting quantum dots, hard discs, Nano-Electro Mechanical Systems (NEMS) or biological samples. Imaging can be performed in air, in vacuum, or in liquid. In a Scanning Force Microscope (SFM), a microscopic tip is scanned over the surface of interest and probes the local properties at each pixel of the scan region. Most commonly, a laser-beam deflection system transduces the tip-sample interaction into a macroscopic signal by measuring either the static or dynamic deflection of a micro-mechanical lever, called a cantilever, which incorporates the force sensing tip and is usually manufactured by silicon microfabrication.

Various tip-sample interaction forces can be mapped and thus different properties of the surface can be imaged. A SFM can not only map topography up to atomic resolution, it can also map other sample properties with nanometer scale resolution such as local mechanical properties, materials contrast, or electric and magnetic stray fields emanating from the surface.



ION-TOF GmbH, Germany

ION-TOF is a manufacturer of innovative instruments for surface analysis with different product lines for time-of-flight secondary ion mass spectrometry (TOF-SIMS) and high-sensitivity low-energy ion scattering (LEIS).

Today, the company, which was founded in 1989, is the leading European manufacturer of time-of-flight secondary ion mass spectrometers and LEIS instruments.

More than 190 tools are in operation in high-tech industries (micro-, nano-, optoelectronics, chemical, glass, display, storage, pharmaceutical, biotechnology etc.), in research centres and at universities.

ION-TOF has a wide range of experience in technology including several relevant patents in the field, expertise in fundamentals of SIMS, instrument design, precision mechanics, high speed electronics and high stability power supplies, software for instrument control and data processing, complete instrument automation and all applications of SIMS.

ION-TOF's success is based on the longstanding SIMS experience and skills of our scientists and engineers, the support given to our customers and the close co-operation with them, and a dedication to supply a good, efficient product to match the demands of the modern users.

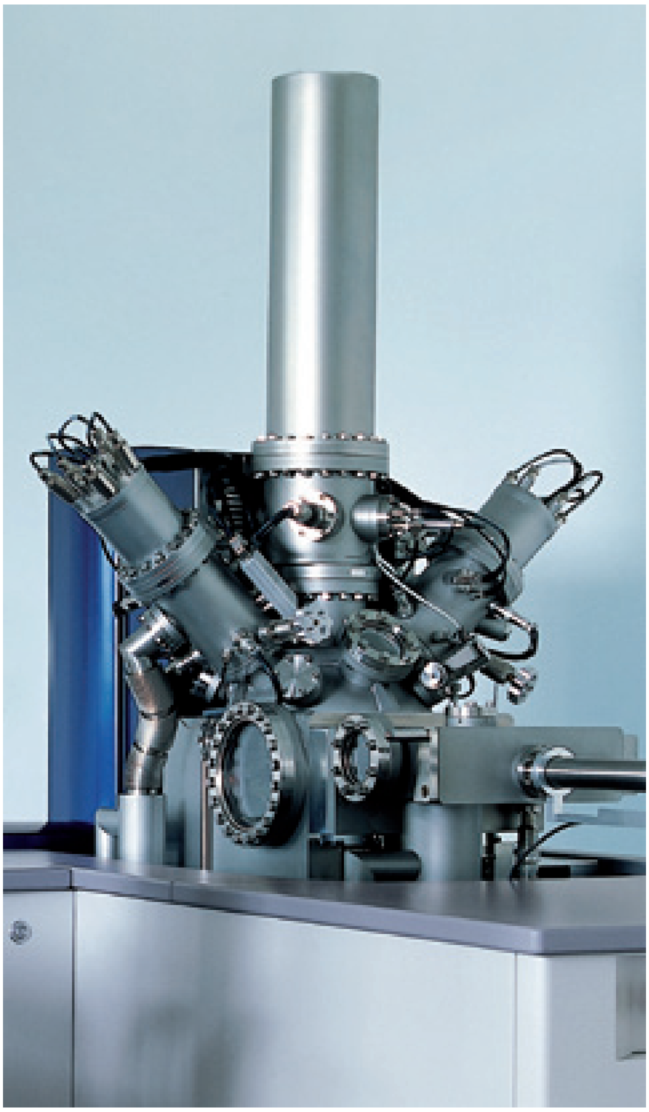
ION-TOF's engineers are not solely involved in developing equipment; basic research is also carried out. Consequently ION-TOF is part of the national German competence centre „Nanoanalytics". The ION-TOF premises are in a science park close to the University, the Technologiehof, the Centre for Nanotechnology (CeNTech) and the Max-Planck Institute for Molecular Biomedicine, which is convenient for collaboration and provides a stimulating working environment.

The involvement in nanoscience projects enables us to understand the instrumental requirements for nanoscience and design them into our instruments. ION-TOF is also an important partner in many other national and international surface science projects.

ION-TOF continues to make considerable development effort. Its policy to build the most innovative ion beam technology for surface science, and the continued investment in the development of our instruments will produce new instruments with even better performance.

Project Contribution

As project co-ordinator, ION-TOF is involved in all work packages and responsible for the project management. The focus of the work is on the instrumental development of ion optical components which will improve the lateral resolution and the sensitivity of the combined TOF-SIMS/SFM instrument. Beyond the TOF-SIMS related developments ION-TOF is responsible for the system integration of the combined tool.



Time-of-flight secondary ion mass spectrometer

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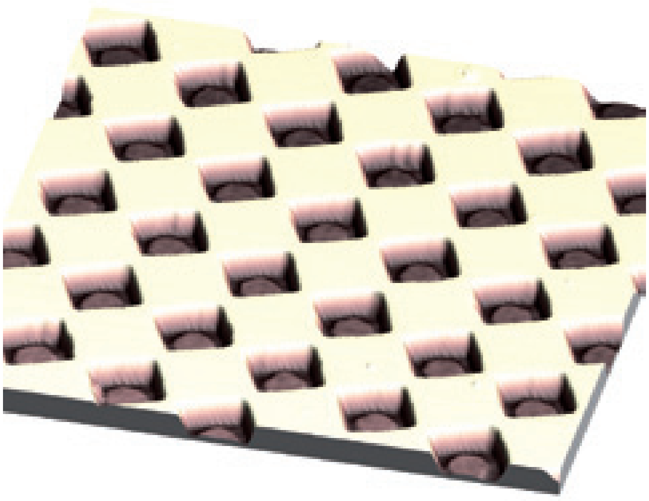
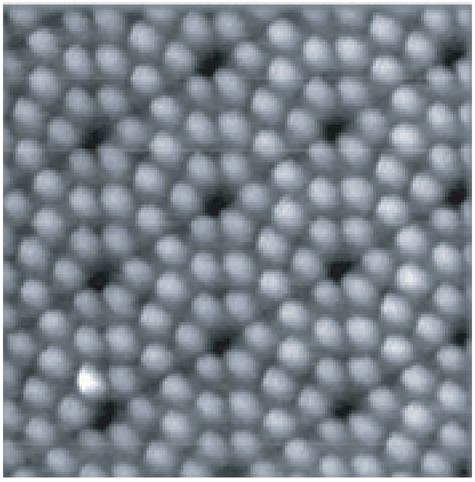
The Eidgenössische Materialprüf- und Forschungsanstalt (EMPA) is a national interdisciplinary research and services institution for material sciences and technology development within the ETH Domain. Empa's research and development activities are oriented to meeting the requirements of industry and the needs of our society, and link together applications-oriented research and the practical implementation of new ideas, science and industry, and science and society. EMPA's key areas of research are grouped into five programs entitled Nanotechnology, Adaptive Materials Systems, Materials for Health and Performance, Natural Resources and Pollutants and Materials for Energy Technologies. Over 800 people work at its three sites in Dübendorf, St. Gallen and Thun.

The EMPA laboratory "Nanoscale Materials Science" is headed by Prof. Dr. Hans Josef Hug and is devoted to the study of the role of the nanoscale composition and structure of materials for their microscopic/macroscopic physical and chemical properties. The improved understanding of the relationship between composition, structure and materials properties then serves as the basis for the design and fabrication of materials with enhanced properties. We perform application use-inspired basic research and make use of our first-class expertise and analytical equipment to be a competent research partner for industry and to offer high-level services to research partners.



AFM micrometric topography of calibration sample (field of view: $12x12um^2$, depth 160nm)

Our interest ranges from the study of atomic and molecular nanosystems by means of advanced scanning probe microscopy (AFM, STM), the development of new scanning probe microscope technology and instruments, (bio)tribology, the fabrication of hard coatings, coatings for medical and industrial applications, magnetic thin films and devices, magnetic shape memory alloys, to surface analysis services by TOF-SIMS, XPS and scanning Auger and nanoscale-3D-mapping of elemental and molecular species by ToF-SIMS.



AFM atomic resolution on Si(111)-7x7 sample (field of view: $5x5nm^2$)

Project Contribution

The role of EMPA in the 3D NanoChemiscope is to design, construct and test (ex-situ) the ultra high vacuum (UHV) SFM instrumentation platform to be integrated into the combined UHV ToF-SIMS/SFM instrument.

The SFM is designed to achieve a lateral resolution of better than 1 nm and a height resolution better than 0.1 nm. Because of the stringent requirement of the tip-sample gap during AFM operation a new high precision, high stability XYZRT piezo-motor stage that includes an AFM scan-head will be developed. The latter uses a capacitively-linearized piezo flexure stage of range 40 x 40 μm^2 to scan the tip relative to the sample. A beam deflection system is used to map the piezo-motor-driven laser cantilever deflection. The XYZRT positioning stage allows reproducible positioning of the sample between the ToF-SIMS and AFM measurement positions. Various operation modes of the SFM will be implemented with emphasis on high speed non-destructive imaging to obtain material contrast with highest spatial resolution.

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NanoScan, Switzerland

NanoScan is Swiss high-tech company founded in 2003 with extensive know-how in the fast-growing field of nanoscience. It focuses on research and development of high-resolution and versatile magnetic and non-contact scanning force microscopes for both industry and academia. Its instruments are designed to fulfil the present and future analytical needs on nanometer-sized surface structures, with a strong emphasis on the best resolution achievable on user-friendly devices.

At present, NanoScan features two versatile Atomic Force Microscopes (AFM):

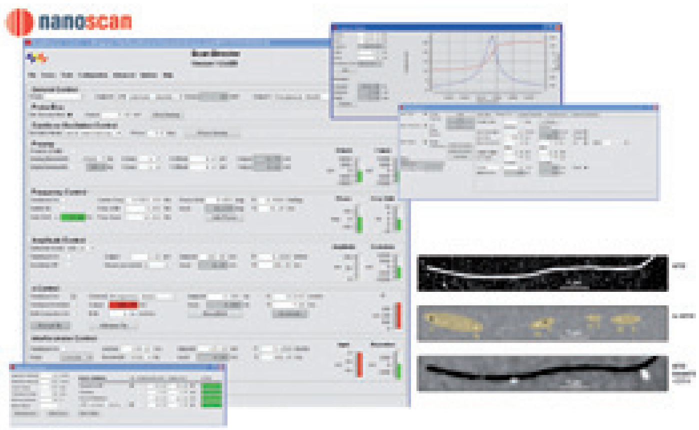
1. The high-resolution Magnetic Force Microscope (hr-MFM) is especially designed for research, development and quality control of magnetic storage media and other magnetic material. It is an analytical and quantitative magnetic imaging system which operates with a fully linearized scanner with a range of up to 40 x 40 µm². The exceptionally high magnetic resolution of 10 nm makes it an excellent tool to analyze surfaces structures and to characterize new magnetic materials and thin-film technology. Additionally, the hrMFM is provided with a positioning system that exhibits a repeatability of 100 nm, and this for sample diameters up to 120 mm.

2. The PPMS®-AFM fits perfectly into the PPMS® (Physical Properties Measurement System) of Quantum Design and is thus only 25 mm in diameter. Joining the AFM with the PPMS provides researchers with a versatile imaging tool in variable temperature (3-390K) and variable magnetic field environment (up to 16T). Despite its dimensions, it offers all common measurement modes such as contact, intermittent, non-contact or high-resolution MFM mode, with a still striking 15-nm magnetic resolution. And the coarse positioning system still allows the user to move the sample over an area of 2 x 2 mm².

These instruments however would not be complete without a tailored controller system. NanoScan developed a proprietary software and control system with the main emphasis on user-friendliness and versatility of the AFM modes. In fact, thanks to its very concepts, the software ScanDirector accommodates to any mode a user may want to implement. As for the control system, a real-time, crash-safe computer monitors all the feedback loops (including a Phase-Lock-Loop) as well as all the scan sequences.

Project Contribution

NanoScan strives to develop innovative concepts in the field of scanning force microscopy. Within the frame of the EU project 3D-NanoChemiscope, it found partners and financial support to carry out an ambitious project: combine the chemical specificity of ToF-SIMS with the topographical information on the nanometer scale of an AFM. The challenge for NanoScan is to design in collaboration with the Empa an Ultra-High-Vacuum-compatible AFM built in the same chamber as the TOF-SIMS, and to develop new features of NanoScan's ScanDirector software. The objective is to produce a new metrological UHV-AFM with a lateral resolution below 1 nm and a vertical resolution below 0.1 nm that can analyze large samples up to 100 x 100 mm². For this, NanoScan uses its know-how gained from the development of its hrMFM.



Detail of NanoScan's software ScanDirector

TOF-SIMS analysis produces craters of a few hundreds of microns in diameter and a few tens of nanometers in depth that the AFM will have subsequently to analyze. Positioning of the crater under the AFM's probe on one hand, and scanning over such large surfaces on the other hand require the development of new modes in ScanDirector. The goal is on one hand to achieve positioning over a range of several centimeters with a precision and a reproducibility of 100 nm and on the other hand to develop a true non-contact mode to a level that the non-expert can easily obtain images, even over ranges that are unconventional in atomic force microscopy (ie over 100 µm).

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PCPM – Université Catholique de Louvain (UCL), Belgium

The research activities concern the physical chemistry of solid surfaces and interfaces. The objective is to develop surface treatments and modifications in order to provide new surface properties for specific applications in materials science. To reach this goal, our approach is based on a control of the surface atomic and molecular composition and structure. The first step required on this road is to be able to characterize the solid surfaces in terms of chemical and functional composition and structure at the nanometer scale. Our main expertise has been the development and the use of surface analytical methods based on the ion-solid interaction, in combination with other surface techniques.

For fifteen years, we have been contributing to the development of the static SIMS technique for the molecular characterization of surfaces, with a special emphasis on organic materials such as polymers or proteins. Current developments are geared towards sub-micrometric 3D molecular imaging with C60 ion sources. The surface properties of interest are biocompatibility, specific catalytic activity, gas/ molecule permeability and adhesion. The methods used to modify the surface are based on chemical and physical treatments.

We have studied surface modification protocols aiming to improve adhesive properties and biocompatibility. A special attention was paid to protein adsorption in view of controlling cell adhesion on micro-patterned polymer surfaces or to prevent biofouling. The group has also built a strong expertise in the field of biosensors, from the synthesis of conducting polymers (polyaniline) to the fabrication and characterization of fully integrated devices.

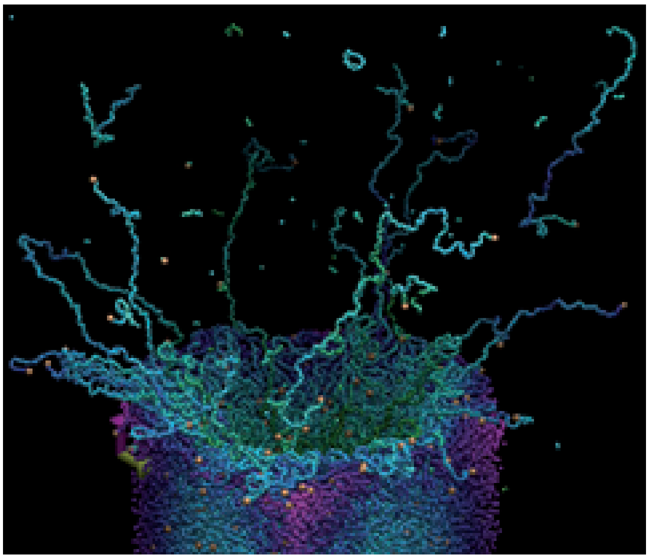
The Main equipment for surface characterization is:

- 2 static imaging time-of-flight mass spectrometers (ToF-SIMS)
- Rutherford Backscatering Spectrometry (using a VDG accelerator) RBS
- Scanning Auger Microprobe (AES–SAM)
- Access to AFM, STM, XPS-ESCA, SEM, TEM, XRD, Ellipsometry, static and dynamic contact angles, IR, Raman
- Access to clean room facilities.

Project Contribution

The PCPM contribution consists in developing new methodologies for organic depth profiling and improving ion yield for atoms and molecules under depth profiling conditions. The depth profiling method employed at PCPM is based on the use of the cluster projectile C60 which features a very low energy per constituent atom.

Fundamental investigations including molecular dynamics simulations provide the basis for new methodological developments. The successful implementation of these tasks also requires the development of reference materials that allow us to perform a systematic evaluation of the organic depth profiling methodologies.



Molecular dynamics simulation of cluster induced sputtering

At the fundamental level, molecular dynamics simulations help us to test bombardment conditions that might be of interest to improve the molecular sputtering yields and organic depth profiling capabilities of SIMS. Various cluster beam species, energies and angles can be considered without the need to setup sometimes costly experimental test sources. These theoretical predictions should indicate the best conditions for organic material sputtering with high yields while at the same time minimizing damage. They serve as a preliminary study for the experimental development of improved primary ion sources in the consortium.

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LISE - University of Namur (FUNDP), Belgium

The LISE laboratory has a 35 years experience in the field of surfaces and interfaces of materials The physicists, chemists and engineers working in LISE have built its international reputation with their research on a large variety of new materials made of complex assemblies of films and particles of different natures. Such research interests industry directly, but as a university laboratory, the main mission of the LISE is also to bring a fundamental understanding on the new properties of those new materials and to their methods of characterization. Two main axes of research can be identified:

Many properties of materials occur essentially at their surfaces, since a material interacts with its environment precisely through its outer layers, or surface. In the same way, the assembly of different materials (polymer-metal, glass-polymer, metal-oxide...) often generates new properties. All the major glass, metal or semiconductor factories develop complex surface treatments, fuelling the need for basic research in this field. The LISE laboratory is equipped with analysis techniques measuring the composition and structure of the matter located at the very surface of a specimen (with an analysed depth of typically 1 nm) or at interfaces, using depth-profiling methods. Those are electron (XPS), ion (ToF-SIMS) and optical spectroscopies, as well as contact angle measurements.

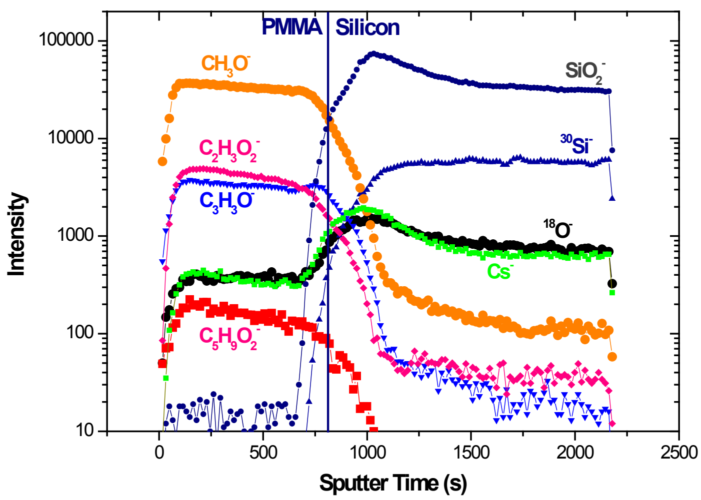
New materials are also produced in the laboratory by plasma techniques (etching, deposition and functionalization) and thin film deposition in vacuum. Recent projects illustrate the large variety of studied problems: coatings for the protection of metals, optical fibers – polymers interfaces, gold nanoclusters on carbon nanotubes, organic light emitting diodes, plasma polymerized thin films ...

The surface analysis techniques are based on the interaction of photons, electrons or ions with matter. However, the fundamentals of those interactions are still poorly understood and scientists in LISE are carrying out some basic research to improve the analytical techniques and their data interpretation. Current research in this field concerns photoemission in nanoparticles, ionisation probability in SIMS, organic matter interaction with ions and application to organic depth-profiling.

Since 2008, the LISE laboratory is part of the Research Centre in Physics of Matter and Radiation (PMR), federating the research activities in the physics department. About 100 people work in PMR, on 70 different projects funded by the EC, the Belgian Federal State, the Walloon Region or industrial partnerships.

Project Contribution

Molecular depth profiling of organic materials was long considered impossible due to the accumulation of radiation damage after the sputter removal of the top surface layer. Recent results presented by LISE researchers demonstrate that true molecular depth profiling of organic layers is possible with reactive ions (caesium or oxygen) at very low sputter energies. An example for 200 eV caesium depth profiling of a 100 nm PMMA polymer film deposited on Silicon is shown below.



200 eV caesium depth profile of a 100 nm PMMA polymer film

LISE will do fundamental investigations on the sputtering of organic materials with ultra low energy sputter ions as an alternative solution to cluster beam depth profiling and develop the respective recipes for optimum depth profiling performance. Crucial parameters such as depth resolution, i.e. interface broadening, are evaluated by means of the reference materials also developed in the project. For the first time sputter energies below 200 eV will be explored for organic materials in this project.

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ISI - Institute of Scientific Instruments AS CR, v.v.i, Czech Republic

The Institute of Scientific Instruments is a research institute of the Academy of Sciences of the Czech Republic (ISI-Brno). It has three major divisions:

- Electron Optics
- Nuclear Magnetic Resonance
- Coherent Optics

The Institute, founded in 1957, has been concerned with instrumental development and design of scientific instruments and some commercial exploitation has emerged from these efforts. More recently, the research is directed to physical methods, special technologies and instrumentation principles used to investigate living and non-living matter.

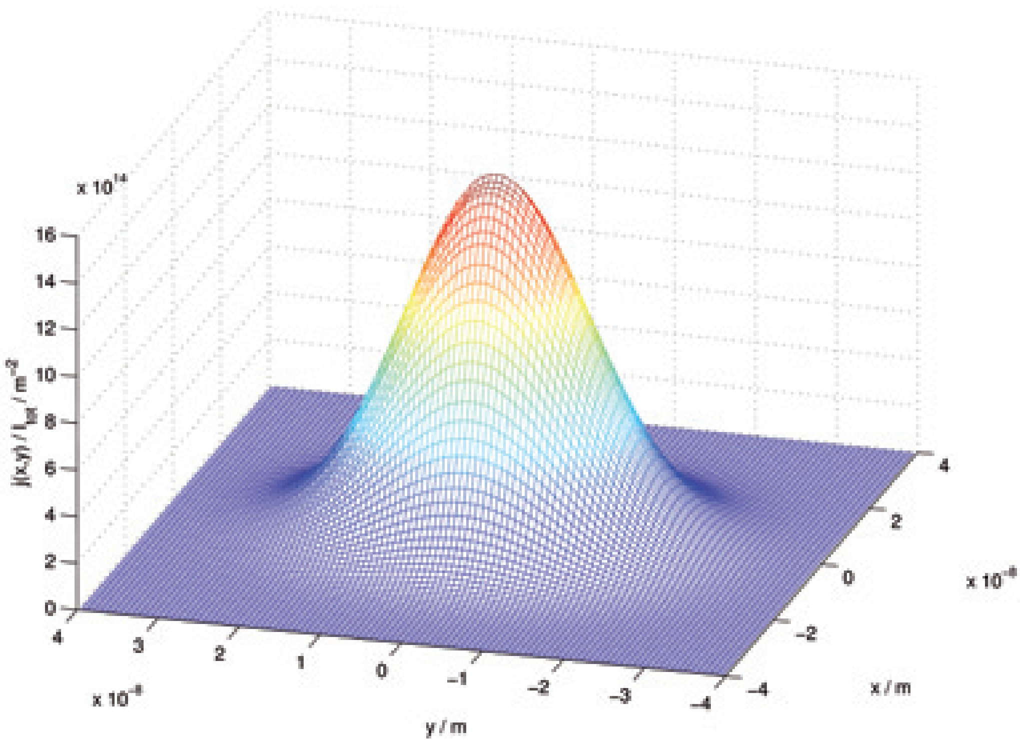
The major efforts of the electron optics department are concentrated on low voltage scanning electron microscopy, detector design, electron beam lithography and special technologies like electron beam welding and micromachining. We also cooperate with universities, research institutions and commercial firms in Czech Republic, European Union and Japan.

The activities of the group of electron optical computer simulations are the development of software and methods for the evaluation of optical properties of devices using charged particles and the support of projects in other groups in the department. Most computations are performed using self developed software based on finite element method for the simulation of focusing and deflection fields and for the evaluation of their optical properties from aberration theory or from accurately traced trajectories of particles. The program EOD that we mostly use has a user-friendly interface for input and output of data and a number of extensions, including the evaluation of space charge effects and coulomb interactions in the beams. We have participated in EU FP5 NANOFIB project (2002-2004) and in a number of projects of Czech grant agencies as well as in grant projects of ISI, TU Brno and Masaryk University.

Project Contribution

The main contribution of ISI-Brno will be the evaluation of properties of ion optical system (electrostatic lenses, beam deflection, mass filter), the evaluation of Coulomb interactions in the ion source and in the column, and improvement of the TOF extraction optics.

Profile of an ion beam



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Holst Centre, The Netherlands

Holst Centre is an independent open-innovation R&D centre that develops generic technologies for Wireless Autonomous Transducer Solutions (WATS) and for Systems-in-Foil (SIF). Holst Centre was set up in 2005 by IMEC (Flanders, Belgium) and TNO (The Netherlands) supported by the Dutch Ministry of Economic Affairs and the Government of Flanders. A key feature of Holst Centre is its partnership model with industry and academia around shared roadmaps and programs. Located on the High Tech Campus in Eindhoven, Holst Centre benefits from the state-of-the-art on-site facilities. This kind of interdisciplinary synergy enables Holst Centre to tune its scientific strategy to industrial needs. Within the SIF program, generic technologies are being developed for the production of flexible organic electronics (OE). Flexible electronics offers distinct advantages over traditional electronics in terms of application areas, design possibilities and free form fabrication, robustness, and cost effectiveness. Low cost production is mainly achieved by the use of cheap and facile manufacturing technologies, such as roll-to-roll printing and coating. Well-known examples of flexible OE devices are organic light-emitting diodes (OLEDs), organic photovoltaic devices (OPVs) (see Figure), as well as organic transistors.

OE devices typically contain multi-layer multi-material stacks of various organic semi-conducting materials. Also transparent inorganic semi-conductors, such as ITO are sometimes used in combination with the organics. Some of these materials, besides being semi-conductive, can also emit light via the creation of so-called excitons. Excitons are electronic distributions representing an energetically elevated state. Upon relaxation of the excited state to the lower-energy ground state the excess of energy is released as a photon. Typically, polymers and small molecules for which this process takes place in a highly efficient fashion are used in OLEDs. During operation, positive charges ('holes') are injected by the anode and electrons are injected by the cathode. The charges travel through the device toward the opposite electrodes. Upon recombination in the active layer the excitons are created, which relax under emission of photons. This way, electricity is converted into light. OPV operate vise-versa by harvesting light and converting it into an electrical current. The active layer of such devices typically contains a blend of p- (donor) and n-type (acceptor) organic semi-conductors. Here, (sun) light is absorbed by the donor material, upon which excitons are formed. The promoted electrons are transferred onto acceptor molecules and, together with the holes left behind on the donor, drained of via the electrodes, thus creating an electrical current.

Flexible OLED (left) and OPV device (right)

Project Contribution

Our task is to supply reference samples for the development of organic depth profiling methodologies based upon SIMS and AFM. These reference samples contain materials and material combinations relevant to the OLED and OPV devices. By these materials, the project will not only create scientific output relating to interfaces of materials which are mainly of academic interest, but also prove the applicability of the 3D NanoChemiscope to interfaces of organic materials having special functionality making them suitable for application in high-tech electronic products. The depth profiling and AFM studies on organic-organic interfaces of OE-related devices have a mutual benefit. They will not only aid the development of new (combined) SIMS and AFM measuring methodologies, but also increase the know-how on OLED and OPV device operation.

Perfectly smooth (organic-organic) interfaces are of utmost importance to optimize the organic depth profiling process. For this reason, we use spin coating as the preferred application method for sample preparation. In a second step we will supply printed multi-layer structures to study the influence of the application methodology on the nature of the organic-organic interfaces.

As an ultimate goal, complete OLEDs and OPV device stacks will be studied using the new combined SIMS/AFM tool.

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The Vienna University of Technology (TU Vienna) lies in the heart of Europe and in close proximity to many important cultural institutions. It was founded in 1815 as a royal-imperial institute. Today, it is the largest technical, scientific education and research institution in Austria, and it is rated as one of the best technical universities of Europe. The TU has an important national and international impact in the field of research. Fundamental research work, the high quality of the research results as well as its close cooperation with commercial companies make the TU one of Europe's leading research universities.

The group of Prof. Hutter works in the field of SIMS since 1978. Primarily using a dynamic sector field instrument, since 2007 the group operates a TOF-SIMS. The group works on the development of new sophisticated TOF-SIMS measurement methods as well in the application of TOF-SIMS for challenging technological tasks.

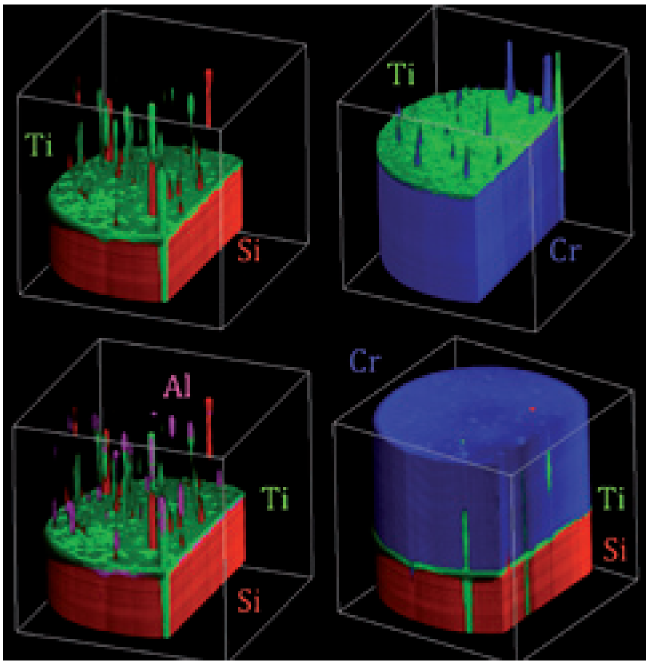
The main contributions to basic science in the field of TOF-SIMS are:

- The investigation of the generation of mass spectra of highly defined organic surfaces (pure polymers, Langmuir Blodgett films, Self organizing monolayers) under Bin^+ (n = 1 to 7) Cluster Ions bombardment.
- Investigating and reduction of the field driven migration of light mobile ions in thin isolating layers during depth profiling. Therefore the group development the soft, field driven incorporation of the light ions into insolating layers.
- Thermodynamic and field driven diffusion of oxygen in oxides by isotope labeling experiments using $^{18}O_2$ (see fig. A).
- Development of new advanced visualization techniques of 3D TOF-SIMS data.

Due to the unique analytical performance of TOF-SIMS the group of Prof. Hutter is additionally active in diverse technological driven tasks:

- Quantitative measurements of H-distribution in semiconductor devices (in cooperation with Infineon), consisting of a stack of conducting and non-conducting layers.
- Oxidation of hard coatings using isotope enriched $^{18}O_2$ and $H_2{}^{16}O$. This investigation will clear up the influence of vapor to the oxidation process and therefore the life time of cutting tools and indicates a pathway to new advanced tribological layer designs.
- Oxygen grain boundary diffusion and selective oxidation of alloying elements in steel.

At the Vienna University of Technology the full range of surface analysis methods are available, e.g.: AES, TEM, XPS and SFM. The group of Prof. Hutter operates an IONTOF TOF-SIMS V and of course, the additional necessary supporting equipment is also present, e.g.: a Digital Holographic Microscope (Lyncee Tec DHM R1101) for 3D optical topography with sub nm depth resolution.



0,5 µm CrN layer on silicon wafer with a 10 nm Ti intermediate layer for improved adhesion

Project Contribution

TU Vienna will develop a data evaluation module (3D Scope) to extract the desired 3D information from the raw data of the SFM and the ToF-SIMS. The calculation of the 3D information requires a perfect overlap of the SFM images and the ToF-SIMS images. An algorithm will be developed to calculate the transformation of the coordinate systems, which is required to match both types of images. Additional algorithms will be necessary to determine the local sputter rates, calculate the correct volume data topography and to correct artifacts introduced by the 3D SIMS measurements. The combined SFM and TOF-SIMS data will be visualized in 3D based on the state of the art computer graphics application VTK.

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