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# **Abbreviations**

AE5	Aug	er e	electro	on spectro	scopy
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AFM	Atomic	force	microsc	эру

DCMS	Direct current magnetron	sputterina

DFT	Density functional theory
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**EVAP** Evaporation

**CU** Comenius University in Bratislava

**EL** Ellipsometry



FIB Focus ion beam

**ISS** Ion scattering spectroscopy

**HiPIMS** High power impulse magnetron sputtering

**HiTUS** High target utilisation sputtering

MD Molecular Dynamics

MUNI Masaryk University in Brno

**NI** Nanoindentation

NTIS New Technologies for the Information Society - European centre of

excellence

**OP** Optical Profilometry

**PLD** Pulsed Laser Deposition

**PVD** Physical vapor deposition

**QMC** Quantum Monte Carlo

**PPMS** Physical Properties Measurement System

**R&D** Research and development

**R&I** Research and innovation

**RS** Raman Spectroscopy

**ScT** Scratch test

**SEM** Scanning electron microscopy

**SP** Spectrophotometry

**TGA** Thermal gravimetric analysis

**TT** Tribology testing

**UPS** Ultraviolet photoelectron spectroscopy

**WDS** Wave dispersive X-ray spectroscopy

**XRF** X-ray Fluorescence

**XPS** X-ray photoelectron spectroscopy

**XRD** X-ray diffraction

**WBU** University of West Bohemia in Plzeň



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# **Executive summary**

In today's competitive landscape, the development and application of advanced materials define the boundaries of innovation across industries. Thin films and coatings have become indispensable in delivering enhanced performance, durability, and functionality to products and systems. To address the growing complexities and demands of modern applications, a comprehensive suite of technologies and services tailored to the needs of industry partners is needed.

Masaryk University in Brno (MUNI), Comenius University in Bratislava (CU), and West Bohemian University in Plzeň (WBU) offer a range of advanced technologies and research capabilities in the field of materials science, specifically focusing on thin films, coatings, deposition technologies, analytical methods and first-principle modelling. Our institutions provide cutting-edge solutions in the following areas:

- 1. Thin Films and Coatings Processing Technologies. We offer a diverse set of deposition techniques, designed to provide precise and versatile solutions for various applications. These methods cater to specific material and surface requirements, enhancing the efficiency and effectiveness of thin films and coatings in industrial and research settings.
- 2. Diagnostics of Deposition Processes. Real-time monitoring technologies are available to ensure the consistent and reliable performance of deposition processes. These systems provide vital data that support process optimization, ensuring high-quality output and minimizing errors during production.
- 3. Morphological Analysis of Surfaces. We utilize advanced imaging and analysis



techniques to offer detailed insights into the morphology of surfaces. This analysis helps to optimize material properties, leading to better functionality and enhanced performance of thin films and coatings in diverse applications.

- **4. Compositional and Structural Characterization.** Through sophisticated techniques, we are enabled the in-depth characterization of material composition and structure. This service aids in supporting innovation and ensuring quality control, particularly in the development and production of high-performance coatings and films.
- 5. Analysis of Physical Properties. We evaluate a range of material properties, including mechanical, electrical, optical, and thermal characteristics, to ensure that materials meet the specific needs of their intended applications. This evaluation process is critical for ensuring the suitability of thin films and coatings in various industries, including electronics, energy, and aerospace.
- **6. First-principle Modelling of Materials.** Utilizing advanced computational modelling techniques, we offer first-principles simulations to predict the behavior of materials. This modelling accelerates the development of new coatings and thin films by enabling researchers to simulate material properties before physical testing, reducing development time and costs.

Our solutions are built on a foundation of **professionalism**, **precision**, **and quality**, ensuring every project meets the highest standards of excellence.

Our approach is defined by **flexibility**, allowing us to adapt to the unique challenges and goals of each partner. Whether developing solutions for cutting-edge research or scaling technologies for industrial applications, we are committed to fostering collaboration and delivering results that exceed expectations.

Partner with us to unlock the potential of advanced thin film and coating technologies. Together, we can create materials and processes that drive **innovation**, **efficiency**, **and success** in your industry.

# **Keywords**

Physical vapor deposition techniques, process control, plasma diagnostics, surface analysis, compositional and structural analysis, mechanical properties, tribological properties, optical properties, thermal analysis, computational modelling of materials.



# 1 COLOSSE technologies and research capabilities

### 1.1. Thin Films and Coatings Processing Technologies

We are pleased to offer a comprehensive suite of Physical Vapor Deposition (PVD) technologies for the preparation of thin films and coatings tailored to meet the demands of cutting-edge industrial and research applications. Leveraging our deep scientific expertise and innovative approach, we specialize in the design, optimization, and transfer of deposition procedures from lab-scale experimentation to industrial-scale production. Our portfolio of PVD methods includes:

#### **Conventional Magnetron Sputtering**

Conventional magnetron sputtering is a widely used physical vapor deposition (PVD) technique in which a target material is bombarded by energetic ions in a magnetic field, causing atoms to be ejected and deposited onto a substrate. This method is commonly employed to create thin films and coatings with controlled thickness and composition in various applications like semiconductor manufacturing and surface engineering.

- **Advantages**: Highly versatile and suitable for uniform coatings on large surfaces; precise control over film thickness and composition; capable of depositing a wide range of materials, including metals, alloys, and ceramics.
- **Applications**: Electronics, optics, and protective coatings.

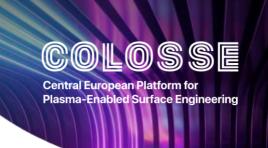
#### High-Power Impulse Magnetron Sputtering (HiPIMS)

High-Power Impulse Magnetron Sputtering (HiPIMS) is an advanced sputtering technique that applies high-power, short-duration pulses to the target material, resulting in increased ionization of the sputtered species. This leads to the deposition of high-quality, dense, and strongly adherent thin films with improved material properties, often used in applications like wear-resistant coatings and semiconductors.

- Advantages: Produces dense, high-quality films with excellent adhesion; enhances ionization for improved coating properties; ideal for complex geometries and hard coatings.
- Applications: Hard coatings, decorative coatings, and tribological applications.

#### Evaporation (Thermal and Electron Beam)

Evaporation is a PVD method where material is heated to a high temperature (using thermal



or electron beam sources) until it vaporizes and condenses onto a cooler substrate to form a thin film. Thermal evaporation uses resistive heating of the material, while electron beam evaporation directs high-energy electrons to the target to achieve higher temperatures, allowing for the deposition of a wider range of materials.

- **Advantages**: Simplicity and high deposition rates; ideal for pure metal and dielectric films; suitable for high-vacuum environments.
- **Applications**: Optical coatings, thin-film solar cells, and reflective surfaces.

#### Pulsed Laser Deposition (PLD)

Pulsed Laser Deposition (PLD) is a thin-film deposition technique where a high-power laser pulse is focused onto a target material, causing it to vaporize and form a plasma that is deposited onto a substrate. This method allows for precise control over the composition and stoichiometry of the thin films, making it ideal for complex materials and high-performance coatings.

- **Advantages**: Excellent stoichiometric transfer of complex materials; capable of depositing multi-layered and functional thin films; ideal for research and development of novel materials.
- Applications: Functional materials, superconductors, and nanostructured coatings.

#### ARC (Cathodic Arc Deposition)

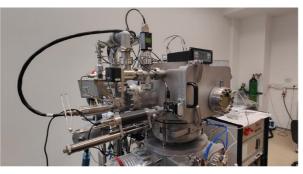
Cathodic Arc Deposition (ARC) is a PVD technique in which an electric arc is generated between a cathode target and an anode, causing the target material to vaporize and ionize, forming a plasma that deposits onto a substrate. This method is commonly used for producing hard, wear-resistant coatings, as well as for metal, ceramic, and composite thin films.

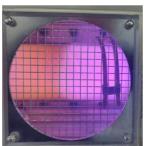
- Advantages: Produces extremely dense coatings; excellent for hard and wearresistant coatings; high deposition efficiency and strong film adhesion.
- Applications: Cutting tools, wear-resistant surfaces, and decorative applications.

#### Scientific Approach to Deposition Procedure Design

The development of high-performance thin films and coatings is critical in applications that require material properties such as enhanced durability, optical clarity, thermal resistance, or electrical conductivity. However, ensuring uniformity, consistency, and quality throughout the production process requires advanced processing techniques and comprehensive measurement and analysis capabilities. Our solution integrates state-of-the-art deposition methods with sophisticated diagnostic tools, enabling real-time monitoring, precise characterization, and optimization of coatings.







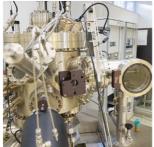




Fig. 1 Lab-scaled physical Vapor Deposition (PVD) technologies for the preparation of thin films and coatings.

Our team takes a **scientific, data-driven approach** to the development and transfer of deposition procedures. We bridge the gap between laboratory-scale precision and industrial-scale productivity by:

- **Optimizing Reactive Processes**: Ensuring controlled and stable reactions to produce high-quality films, especially in reactive sputtering and arc processes.
- **Achieving Uniform Coverage**: Designing solutions for uniform deposition on complex-shaped components and substrates.
- **Improving Target Utilization**: Enhancing yield and cost-effectiveness by minimizing waste and maximizing target material use.
- **Scaling Up**: Developing deposition protocols that translate seamlessly from research equipment to large-scale industrial systems.
- **Customizing Equipment Modifications**: Collaborating with partners to design and implement technological enhancements for existing industrial systems, focusing on improved throughput, process stability, and coating performance.

Our experts in PVD techniques are ready to assist you with your material deposition needs. Feel free to reach out, and our team will provide you with the best solutions tailored to your requirements.



#### 1.2. Diagnostics of Deposition Processes

We are pleasure to offer Diagnostics of Deposition Processes using various techniques and tools to monitor and analyze the conditions and parameters during the deposition of thin films or coatings. These diagnostics help ensure that the process is optimized for uniformity, quality, and desired material properties. Key diagnostics include monitoring the plasma environment, material flux, deposition rate, substrate temperature, and film stress. By providing real-time feedback, these diagnostic methods allow for adjustments during deposition, ensuring high-quality, reproducible films. Our portfolio includes:

- Langmuir Probes: Measure plasma parameters like electron temperature and density, which directly influence film quality during deposition.
- Optical Emission Spectroscopy (OES): Monitors the chemical composition of the plasma, providing insights into process stability and enabling optimization of deposition parameters.
- Mass Spectrometry (MS): For gas phase analysis, helping optimize the selection of precursor gases and improving film quality.

#### **Benefits of Diagnostics of Deposition Processes:**

- **Improved Film Quality**: Diagnostic techniques provide real-time monitoring of the deposition process, allowing for adjustments that ensure better film uniformity, density, adhesion, and optical or mechanical properties.
- **Process Optimization**: By analyzing key parameters such as temperature, pressure, and deposition rate, diagnostics help optimize the process, improving efficiency, reducing material waste, and enhancing throughput.
- **Increased Process Control**: Real-time feedback enables more precise control over film thickness, composition, and microstructure, ensuring that the desired material properties are consistently achieved.
- **Error Detection and Troubleshooting**: Diagnostics help identify deviations or issues in the deposition process, such as target poisoning, substrate contamination, or equipment malfunction, enabling prompt corrective actions to avoid defects.
- Predictive Maintenance: Monitoring deposition parameters can reveal signs of equipment wear or failure, allowing for proactive maintenance and reducing downtime.
- Customization for Specific Applications: Advanced diagnostics enable the finetuning of deposition parameters for specific applications, such as semiconductor manufacturing, optics, or coatings, ensuring that the film meets the exact requirements for each use case.
- **Better Reproducibility**: Continuous process monitoring ensures that deposition conditions are consistent across batches, improving reproducibility and the reliability of the final product.
- Cost Reduction: By ensuring that the process is optimized, diagnostics help reduce



the consumption of materials, energy, and time, leading to more cost-effective deposition.

- **Enhanced Material Performance**: Understanding and controlling the deposition process can lead to films with improved properties such as higher hardness, wear resistance, conductivity, and optical characteristics.
- **Compliance with Standards**: In industries where precise material specifications and quality are crucial (e.g., aerospace, electronics), diagnostics help ensure that films meet regulatory standards and specifications.



Fig. 2. Diagnostics methods of deposition processes.

Overall, diagnostics of deposition processes are essential for ensuring high-quality, efficient, and cost-effective manufacturing, especially in industries requiring precision and reliability.

#### Scientific Approach to Diagnostic of Deposition Processes

The scientific approach to diagnostics in PVD deposition processes focuses on understanding and controlling the physical and chemical phenomena occurring during the deposition. A robust diagnostic methodology is essential for optimizing the deposition conditions, ensuring uniform film thickness, high adhesion strength, and desired material properties. By using a combination of plasma diagnostics, material flux monitoring, and substrate diagnostics, PVD processes can be precisely controlled and optimized. These diagnostic tools provide valuable insights into the complex interactions within the deposition chamber, allowing for real-time process adjustments and ensuring the success of thin film deposition, leading to high-quality, reproducible films with the desired properties across various industries.



Our team is dedicated to delivering **cutting-edge diagnostic solutions** that help you achieve high-quality, reliable, and reproducible thin films and coatings. Whether you are involved in research, development, or large-scale manufacturing, our diagnostics will ensure your deposition processes are efficient, controlled, and of the highest quality.

#### 1.3. Morphological Analysis of Surfaces

We are pleased to offer Morphological Analysis of Surfaces of Thin Films and Coatings, which involves studying the microstructure, fracture, and topography of a thin film or coating's surface at various scales. This analysis provides valuable insights into the film's growth patterns, roughness, uniformity, and any defects or irregularities that may impact its performance. Common techniques we use for morphological analysis include:

- **Atomic Force Microscopy (AFM):** Offering high-resolution, nanoscale imaging to measure surface roughness, texture, and detect any defects.
- **Scanning Electron Microscopy (SEM):** Providing detailed, high-magnification images of surface morphology, revealing film quality, grain structure, and surface features.
- **Optical Profilometry (OP):** A non-contact method for measuring surface topography and generating 3D maps of the film surface.

#### **Benefits:**

The Morphological Analysis of Surfaces of Thin Films and Coatings offers several key benefits that are critical for optimizing film quality and ensuring performance in various applications:

#### **Quality Control and Consistency**

- **Uniformity Assessment:** Morphological analysis helps identify surface irregularities, roughness, and non-uniformities that could affect the film's functionality, ensuring that the coatings meet strict quality standards.
- **Defect Detection:** It enables the detection of defects such as cracks, pinholes, and voids that could compromise film integrity and performance.

#### **Optimization of Deposition Processes**

- **Growth Pattern Analysis:** By examining the surface structure and texture, the analysis provides insights into the growth mechanisms of the film, helping to optimize deposition parameters for desired properties.
- **Process Fine-Tuning:** Helps identify correlations between deposition parameters (e.g., temperature, pressure, material flux) and film morphology, enabling better control over film characteristics.



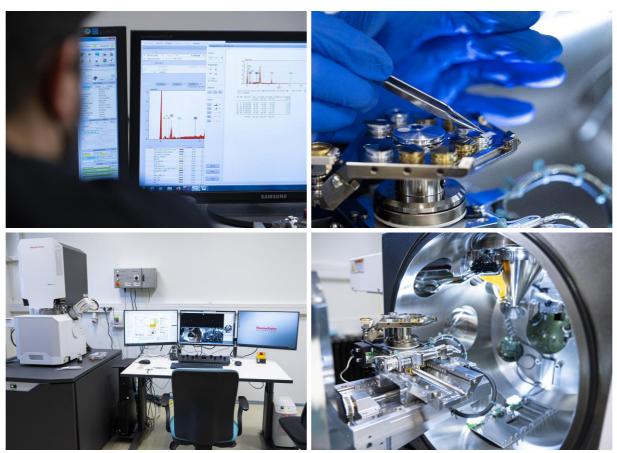


Fig. 3. Morphological analysis of thin films and coatings using Scanning electron microscopy.

#### **Enhanced Film Performance**

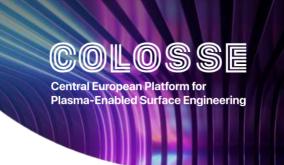
- **Surface Properties Improvement:** Understanding the surface morphology aids in modifying roughness or texture, improving adhesion, mechanical strength, and wear resistance of the coatings.
- **Interface Quality:** Ensures good adhesion between the film and substrate, which is crucial for applications where bonding strength is critical, such as in electronics and aerospace.

#### **Nanoscale Precision**

 High-Resolution Imaging: With techniques like Atomic Force Microscopy (AFM), morphological analysis offers nanoscale imaging, allowing for precise measurements of features like grain size and surface roughness that are critical for advanced technological applications.

#### **Cost and Time Efficiency**

• Non-Destructive Testing: Techniques such as AFM and SEM allow for detailed



- surface analysis without damaging the film, ensuring that the coatings can be tested and analyzed during various stages of production.
- **Real-Time Monitoring:** With rapid analysis, morphological measurements help detect process deviations early, saving time and reducing material waste.

#### **Customization for Specific Applications**

• **Tailored Coating Design:** Depending on the application, whether in optics, electronics, or protective coatings, morphological analysis helps design films with specific surface features, such as enhanced smoothness or roughness for better optical or mechanical properties.

#### Scientific approach to morphological analysis of surfaces of thin films and coatings

The scientific approach to morphological analysis of surfaces of thin films and coatings is a comprehensive process that combines advanced techniques to study the film's structure, roughness, grain morphology, and topography. This analysis is crucial for ensuring that thin films meet the required specifications for various applications, ranging from electronics and optics to protective coatings. By linking the morphological features with functional properties, this approach not only helps optimize deposition processes but also ensures the reliability and performance of thin films in their intended applications.

Our team combines advanced analytical techniques with expertise to help you optimize deposition processes, improve material properties, and ensure consistent, high-quality results. We offer:

- **Expertise and Precision:** combination of years of experience with advanced diagnostic techniques to provide accurate, reliable morphological analysis.
- **Comprehensive Solutions:** a wide range of analytical tools and expertise, enabling a thorough understanding of your thin films and coatings across multiple scales.
- **Customization for Your Needs:** tailoring of our analysis to meet the specific requirements of your applications, whether in research, development, or large-scale production.
- **Optimized Film Performance:** By correlating morphological characteristics with functional properties, we help ensure that your thin films and coatings perform at their best.

We are committed to delivering high-quality, detailed, and actionable insights into your thin films and coatings, empowering you to optimize your deposition processes and achieve superior results.



#### 1.4. Compositional and Structural Characterization

Compositional and Structural Characterization of thin films and coatings refers to the analysis of both the chemical composition and the physical structure of the material. These characterizations are essential for understanding how the material's properties are influenced by its elemental makeup and internal structure, which ultimately affects its performance in various applications. We offer:

Compositional characterization focuses on identifying and quantifying the elements and compounds present in a thin film or coating. This analysis is critical for ensuring that the material meets specific requirements, such as purity, stoichiometry, or the presence of alloying elements.

#### **Key Techniques for Compositional Characterization**

- X-ray Photoelectron Spectroscopy (XPS): XPS analyzes the surface composition of thin films by measuring the binding energies of core electrons ejected from atoms when exposed to X-rays. It provides detailed information about the chemical elements present, their oxidation states, and the chemical environment of the surface.
- Energy Dispersive X-ray Spectroscopy (EDS): Often used in conjunction with Scanning Electron Microscopy (SEM), EDS detects X-rays emitted from a specimen when bombarded by an electron beam, providing elemental composition information. Used for surface and bulk analysis, offering elemental mapping of films and coatings, as well as quantifying the composition.
- Wavelength Dispersive X-ray Spectroscopy (WDS) is an advanced technique used for elemental analysis of materials, particularly in thin films and coatings. It involves the detection and measurement of X-rays emitted by a sample when it is bombarded with electrons. WDS is commonly used in conjunction with scanning electron microscopy (SEM) for surface analysis, offering detailed compositional insights in materials science, electronics, and coatings.
- X-ray Fluorescence (XRF): XRF detects the characteristic X-rays emitted when a material is exposed to high-energy X-rays. It provides information about the elemental composition. Non-destructive method for elemental analysis, particularly useful for bulk and surface composition without altering the sample.

Structural characterization focuses on understanding the internal arrangement, phase composition, and crystallinity of the material. This type of analysis is important for assessing how the film's structure influences its mechanical, electrical, thermal, and optical properties.

#### **Key Techniques for Structural Characterization**

• X-ray Diffraction (XRD): XRD measures the diffraction patterns produced when X-rays are directed at the sample. These patterns provide information about the



- crystalline structure of the material. Used to identify phase composition, crystallinity, grain size, and crystallographic orientation. It is essential for determining the structure of thin films, whether amorphous or crystalline.
- Raman Spectroscopy (RS): Raman spectroscopy measures the vibrational modes
  of a material when it is exposed to laser light, providing information about molecular
  and crystal structures. It helps identify phases, stress, and defects in thin films.
   Raman can be used for both crystalline and amorphous materials and can provide
  insight into film uniformity.

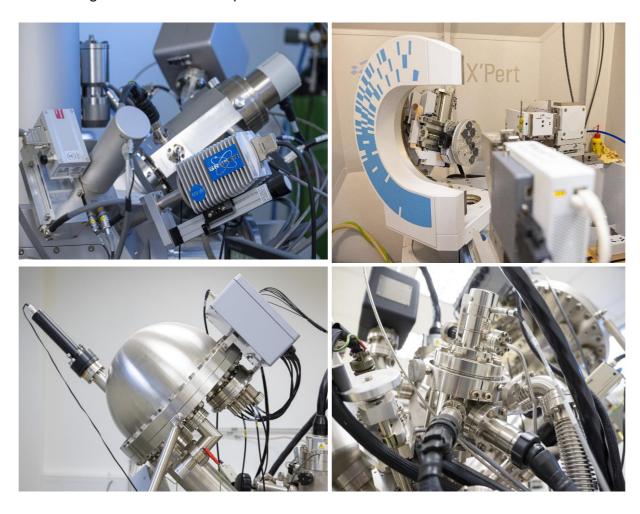
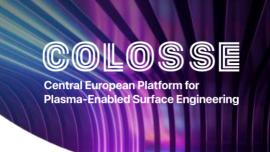


Fig. 4. Compositional and structural analysis of thin films and coatings by means of X-ray spectrometry and X-ray diffraction.

#### **Benefits:**

The Compositional and Structural Characterization of Thin Films and Coatings offers several key benefits that are critical for optimizing film quality based on elemental and structural variations and ensuring performance in various applications:

• **Performance Prediction:** The composition and structure of a thin film directly influence its electrical, optical, mechanical, and thermal properties. Accurate



characterization helps predict how the film will perform in a given application.

- **Process Optimization:** By understanding the material's composition and structure, deposition processes can be fine-tuned to achieve desired properties such as film thickness, adhesion, crystallinity, or defect reduction.
- Quality Control: Routine compositional and structural analysis ensures the thin films
  meet required specifications and performance standards, reducing defects and
  ensuring reproducibility.
- **Material Development:** Characterization helps in the development of new materials with tailored properties, enabling innovations in various fields such as electronics, coatings, solar cells, and more.

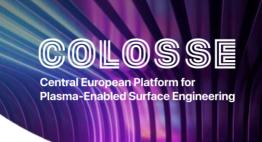
#### Scientific Approach to Compositional and Structural Characterization

The scientific approach to compositional and structural characterization of thin films and coatings involves a combination of advanced techniques to accurately assess the material's elemental quality and quantity and internal structure. This comprehensive analysis provides critical insights into how the material's properties—such as mechanical strength, conductivity, optical performance, and durability—are influenced by its composition and structure.

We are pleased to offer an in-depth analysis of thin films and coatings, helping you optimize material properties and performance. Our services are designed to deliver precise, reliable insights into the composition and structure of your films, ensuring they meet the highest standards for various applications. We offer:

- **Cutting-Edge Technology:** We employ the latest, most accurate analytical techniques to provide detailed, reliable compositional and structural data.
- **Expert Team:** Our team of scientists and engineers has extensive experience in materials characterization, ensuring expert analysis and tailored solutions for your specific needs.
- **Comprehensive Data Analysis:** We offer a holistic approach that integrates both compositional and structural insights to optimize your thin films for enhanced performance.
- Customer-Focused Solutions: We work closely with you to ensure that the characterization results align with your goals, providing actionable insights and recommendations.

We are committed to helping you achieve the highest quality thin films and coatings, offering expert analysis and process optimization to meet your technical requirements and drive success in your applications.



#### 1.5. Analysis of Physical Properties of Thin Films and Coatings

The analysis of physical properties of thin films and coatings is essential for understanding their performance in various applications, such as electronics, optics, and energy devices. We offer a measurement of key properties include:

- **Mechanical Properties** Nanoindentation and scratch tests evaluate hardness, adhesion, and mechanical stability. Tribology measurement (ball-on-disc)
- **Optical Properties** Spectrophotometry (SP) and ellipsometry (EL) measure refractive index, absorption, and transmittance for applications in coatings and photonics.
- **Electrical & Conductive Properties** Four-point probe and Hall effect measurements assess resistivity, conductivity, and carrier mobility. Measurement in magnetic fields.
- **Thermal Stability** Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) assess stability under temperature variations.

By combining these techniques, researchers optimize thin film properties for advanced materials and device applications.

#### **Benefits:**

#### **Mechanical Properties Analysis**

- **Enhanced Durability:** Understanding the mechanical properties (e.g., hardness, tensile strength, elasticity, and fracture toughness) of thin films helps predict their performance under stress and mechanical wear. This is especially important for coatings applied to surfaces that undergo wear, pressure, or friction.
- **Optimized Design:** By assessing the mechanical strength, films can be designed with the required robustness, reducing the risk of failure in real-world applications.
- **Improved Adhesion:** Mechanical testing can reveal the bonding strength between the thin film and the substrate, which is critical for applications such as coatings in semiconductor devices and automotive parts.

#### **Optical Properties Analysis**

- Tailored Optical Performance: The optical characteristics (e.g., reflectivity, transmittance, absorption, and refractive index) of thin films are essential for designing coatings in applications like antireflective coatings, optical filters, and sensors.
- **Light Manipulation:** For applications in photonics and photovoltaics, understanding how thin films interact with light allows for optimization in light harvesting and emission properties.
- Improved Aesthetic and Functional Coatings: Thin films used for decorative or protective coatings often rely on optical properties to achieve desired visual effects



or to improve surface durability.

#### **Electrical and Conductive Properties**

- Conductivity Optimization: Understanding the electrical properties (e.g., resistivity, carrier concentration, and mobility) of thin films allows for the development of coatings and films that optimize the conductivity of semiconductor devices, sensors, and conductive coatings.
- **Device Performance:** For thin films used in electronic components like transistors, resistors, or capacitors, evaluating electrical properties ensures that the film meets the desired performance criteria, such as high conductivity or insulation properties.
- **Temperature Dependence:** Using a Physical Property Measurement System (PPMS), the temperature dependence of electrical conductivity can be evaluated, which is crucial for understanding the behavior of materials in different environmental conditions.

#### **Thermal Stability Analysis**

- **Prevention of Degradation:** Evaluating thermal stability helps predict how a thin film or coating will perform when exposed to high or fluctuating temperatures. This is especially important for applications in aerospace, automotive, and industrial sectors where coatings are subjected to high-temperature environments.
- **Thermal Expansion Matching:** Thin films often experience different rates of thermal expansion compared to the substrate. Analyzing thermal stability helps ensure that there is minimal mismatch, which could lead to delamination or cracking of the film.
- **Long-term Reliability:** Understanding the degradation or changes in properties due to thermal cycling or exposure to extreme temperatures is essential for ensuring the longevity and reliability of thin films in real-world applications.

#### **Improved Performance and Application Suitability**

- Customizing for Specific Applications: Detailed analyses of physical and thermal properties enable the customization of thin films for specific applications. For example, coatings used in microelectronics need to have high thermal stability and conductivity, while those used in optics require low absorption and high transparency.
- **Better Material Selection:** Comprehensive property analysis helps in the selection of the right materials for thin films and coatings, ensuring they meet the necessary requirements for specific devices or systems.
- **Enhanced Manufacturing Processes:** Insights from these analyses can inform the optimization of deposition processes (e.g., sputtering, CVD, etc.), allowing to produce films with desirable characteristics.



#### **Enhanced Predictive Capability and Quality Control**

- **Failure Prediction:** By examining properties like mechanical strength and thermal stability, it's possible to predict failure modes under various environmental conditions, leading to better design and quality control of products.
- Advanced Simulation and Modelling: Data on these properties can be fed into simulation tools to predict the behavior of films and coatings in real-world applications, improving product development cycles and reducing the need for trial-and-error testing.

In summary, analyzing these properties provides valuable insights that help improve the performance, durability, and reliability of thin films and coatings, making them suitable for high-performance applications across industries such as electronics, optics, automotive, and energy.



Fig. 5. Analytical methods of physical properties characterization of thin films and coatings.

#### Scientific Approach to Analysis of Physical Properties of Thin films and Coatings

A scientific approach to analyzing the physical properties of thin films and coatings involves a combination of experimental techniques, data analysis, and modelling to understand their behavior under various conditions. This comprehensive understanding helps in designing films with optimized properties for specific applications in electronics, optics, energy, and materials science. The goal is to obtain reliable, reproducible results that can guide material selection, process optimization, and application-specific modifications for high-performance films and coatings.



We offer a comprehensive and scientifically-based approach to measure the physical properties of thin films and coatings, utilizing state-of-the-art techniques to ensure accurate, reliable, and reproducible results. Our services are designed to help you optimize the performance, durability, and quality of your thin films and coatings, whether for research, development, or industrial applications. We offer:

- **Advanced Equipment:** We use cutting-edge tools and techniques to ensure precise measurements.
- **Scientifically-Validated Approach:** Our methods are based on well-established scientific principles and industry standards.
- **Expert Team:** Our team of experienced researchers and engineers provides detailed insights into your materials' behavior.
- **Comprehensive Reports:** Receive clear, actionable data along with expert analysis and recommendations for material optimization.

Contact us for more details or to schedule your physical property measurement services. Optimize the performance and reliability of your thin films and coatings with our scientific approach.

#### 1.6. First-principle Modelling of Materials

**First-Principles Modelling of Materials** services to predict and optimize the behavior, properties, and performance of materials at the atomic and molecular level. Leveraging advanced computational methods based on quantum mechanics, our services provide deep insights into material design, development, and performance prediction, all with high accuracy and scientific rigor. Our Offer Includes:

#### Density Functional Theory (DFT) Calculations

- **Electronic Structure Analysis**: Study the electronic band structure, density of states (DOS), and charge density distribution. This helps in understanding conductivity, optical properties, and more.
- Bonding and Reaction Pathways: Identify and analyze atomic interactions, molecular bonding, and reaction pathways for catalysis, surface reactions, and phase transformations.
- **Defect and Impurity Analysis**: Investigate the impact of defects, doping, and impurities on material properties such as electrical conductivity, magnetism, and thermal properties.

#### Molecular Dynamics (MD) Simulations

• **Atomistic Simulations**: Model the time-dependent behavior of materials to predict their thermodynamic properties, diffusion mechanisms, and mechanical responses



at the atomic level.

- **Thermal and Structural Stability**: Simulate the material's response to thermal fluctuations, including phase transitions, melting points, and material degradation.
- **Elasticity and Fracture**: Study the material's mechanical response to stress, strain, and deformation, as well as predict failure modes.

#### Quantum Monte Carlo (QMC) Simulations

- **Highly Accurate Energy Calculations**: Use QMC to calculate the most accurate ground-state energy and properties for systems where DFT might not provide sufficient precision.
- **Electron Correlation Effects**: Account for many-body electron correlations that are difficult to capture with conventional methods, making it particularly useful for strongly correlated materials.

#### **Phonon and Vibrational Analysis**

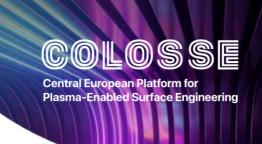
- **Vibration Modes**: Study phonon dispersion curves, vibrational frequencies, and thermal properties using first-principles calculations.
- **Thermal Conductivity**: Predict and optimize thermal transport properties by analyzing phonon scattering mechanisms.
- **Material Properties at Extreme Conditions**: Simulate materials under extreme pressures and temperatures, such as in high-performance aerospace or energy applications.

#### **Materials Design and Screening**

- **Materials Discovery**: Identify novel materials with desired properties, such as superconductivity, high thermal stability, or optimal conductivity, by screening large databases of compounds using first-principles methods.
- **High-Throughput Virtual Screening**: Perform rapid screening of thousands of candidate materials to predict their properties, enabling faster development cycles.
- **Multi-Scale Modelling**: Integrate first-principles results with larger-scale simulations (e.g., continuum mechanics, mesoscopic models) for a more comprehensive materials design process.

#### **Interface and Surface Modelling**

- **Surface and Interface Studies**: Model the atomic structure, energetics, and properties of surfaces and interfaces, which are critical in thin films, coatings, catalysts, and semiconductor devices.
- **Adsorption and Catalysis**: Predict adsorption energies, reaction mechanisms, and catalytic performance for materials used in energy storage, fuel cells, and catalysis applications.



#### **Magnetic and Optical Properties**

- **Magnetic Materials**: Simulate magnetic behavior and magnetic interactions in materials, such as ferromagnetism, antiferromagnetism, and spintronic properties.
- Optical Properties: Predict optical absorption spectra, dielectric constants, and refractive indices, useful in the design of optoelectronic devices, such as solar cells and LEDs.

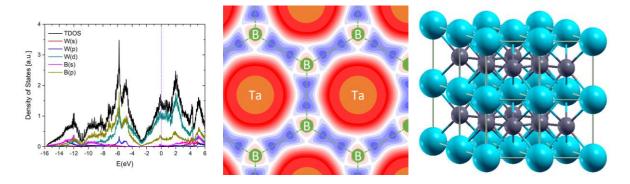


Fig. 6 First-principle modelling of materials – examples of outputs.

#### **Benefits:**

- Accurate Predictions: Based on quantum mechanics, first-principles modelling
  offers precise predictions of material properties without needing experimental data,
  ensuring high accuracy and reliability.
- **Material Discovery & Design:** It enables the discovery of new materials and the optimization of existing ones for specific applications, such as electronics, energy storage, and catalysis.
- Cost and Time Efficiency: By simulating material behavior at the atomic level, first-principles modelling reduces the need for expensive and time-consuming physical experiments, speeding up development cycles.
- **In-Depth Insights:** Provides detailed understanding of atomic, electronic, and mechanical properties, helping identify novel phenomena and predict material behavior in extreme conditions.
- **Customized Applications:** Allows for the design of materials with tailored properties, such as high conductivity, strength, or thermal stability, for specific industries like aerospace, energy, and semiconductors.
- **Surface and Interface Analysis:** Accurately models the behavior of materials at surfaces and interfaces, critical for coatings, and thin films.
- **Multi-Scale Integration:** Integrates atomic-scale insights with higher-scale models to simulate real-world material behavior under practical conditions.
- **Environmental and Sustainability Benefits:** Helps develop eco-friendly, energy-efficient materials by simulating their properties and environmental impact.
- Complex Systems Understanding: Useful for studying complex materials, alloys,



and quantum systems, providing insights that traditional methods can't achieve.

• **Machine Learning Integration:** Complements machine learning approaches for faster material discovery and predictive analytics in material design.

First-principles modelling accelerates material innovation, providing deep insights and reducing costs, making it an essential tool for modern materials science.

#### Scientific Approach to First-principles modelling

First-principles modelling, also known as ab initio modelling, is based on quantum mechanical principles to predict the properties of materials without empirical parameters. It primarily relies on solving fundamental equations of quantum mechanics to understand material behavior at the atomic and molecular scale.

We offer comprehensive **first-principles modelling** services to help you understand and optimize the properties of materials at the atomic level. Our offer includes **State-of-the-Art Methods**; **High-Performance Computing**; **Expert Team**; **Cost and Time Efficiency**; **Comprehensive Reports**.

Unlock the full potential of your materials with our **first-principles modelling services**. Whether you're designing new materials, optimizing existing ones, or exploring new applications, our advanced simulations can accelerate your research and development. Contact us to discuss your specific needs and how we can help you achieve your material design goals with precision and efficiency.



#### Summary table of technologies, analytical methods and modelling approaches

		Masaryk University in	Comenius University	West Bohemian
	Abbrevaition	Brno	in Bratislava	University in Pilsen
Thin Films and Coatings Processing Technologies				
Cathodic evaporation	ARC		•	
Evaporation	Evap	V•	•	
Direct current magnetron sputtering	DCMS		•	•
High power impulse magnetron sputtering	HiPIMS	•	•	•
High target utilisation sputtering	HiTUS		•	
Pulsed Laser Deposition	PLD		•	
Diagnostics of Deposition Processes				
Langmuir Probes		•		•
Mass Spectroscopy	MS			
Optical Emmision Spectroscopy	OES	•		•
Morphological Analysis of Surfaces				
Atomic force microscopy	AFM		•	
Focus ion beam	FIB			
Optical Profilometry	OP		•	
Scanning electron microscopy	SEM	•	•	1
Compositional and Structural Characterization	OE.III			
Auger electron spectroscopy	AES	1		
Energy dispersive X-ray spectroscopy	EDS		•	
lon scattering spectroscopy	ISS	•	•	•
	2 (		•	
Raman Spectroscopy	RS	•		• >
Ultraviolet photoelectron spectroscopy	UPS	•	•	
Wave dispersive X-ray spectroscopy	WDS	•	•	• /
X-ray photoelectron spectroscopy	XPS	•	•	
X-ray Fluorescence	XRF			<b>/•</b>
X-ray diffraction	XRD	•	•	/ •
Analysis of Physical Properties				
Differential scanning calorimetry	DSC			•
Ellipsometry	EL	•	• /	/ ·
Nanoindentation	NI	•	• /	
Physical Properties Measurement System	PPMS		• /	/
Spectrophotometry	SP			
Scratch test	ScT		<b>/•</b> /	
Thermal gravimetric analysis	TGA			
Tribology testing	π		/ •	
Hall measurement system				
Four-point probe			•	•
Rapid thermal annealing	RTA		•	•
Profilometry				
Surface tension				
Chromatography				
First-principle Modelling of Materials				
Density functional theory	DFT			
Molecular Dynamics	MD	5704	107001	
Quantum Monte Carlo	QMC	•	•	
Quartar Hyorice Carlo	QIVIC		•	•



#### 2 Outlook

As industries evolve and demand more advanced materials, the technological landscape for thin films, coatings, and materials science is set for significant growth and innovation. The initiatives from **Masaryk University**, **Comenius University**, **and West Bohemian University** exemplify a forward-looking approach to addressing the challenges of modern material development.

We foresee precise, **adaptable PVD deposition techniques** like HiPIMS playing a pivotal role in meeting the diverse needs of industries such as electronics, energy, aerospace, and healthcare. As applications expand, these technologies will enable the creation of highly specialized coatings and thin films, tailored to enhance product performance and longevity.

We anticipate that **the diagnostics of deposition processes** will become increasingly sophisticated with the integration of AI and machine learning. This will allow for real-time, predictive process monitoring and optimization, boosting efficiency while minimizing waste and ensuring the reproducibility of deposition processes, resulting in consistent production runs.

In the field of **morphological surface analysis**, we are confident that future advancements will offer deeper insights into surface interactions, paving the way for the creation of materials with novel properties. These breakthroughs will drive the development of more resilient, efficient, and multifunctional materials across a wide array of applications, from nanotechnology to large-scale industrial processes.

We also expect that the evolution of **compositional and structural characterization** will continue, with increasingly advanced tools enabling more detailed analysis at the atomic and molecular levels. As the demand for innovative materials grows, these techniques will be essential for maintaining rigorous quality control and facilitating the development of cutting-edge materials tailored to the complex needs of emerging technologies.

We believe that **the analysis of physical properties** will remain central to validating material performance. The ability to rapidly assess mechanical, electrical, and thermal properties under various conditions will help industry leaders stay competitive in the fast-evolving materials market. Tailoring material properties will be key to developing next-generation products and systems.

Finally, we are convinced that **first-principles modelling** will become indispensable in accelerating material discovery and design. By simulating material behavior before physical testing, researchers can fast-track the development of new coatings and thin films, cutting costs and reducing time-to-market. As computational power continues to advance, these models will become more accurate and efficient, enabling the creation of materials with precisely engineered properties.

In this dynamic environment, **our institutions are making significant strides to keep pace with these challenges**, continually enhancing their scientific and analytical capabilities. This commitment ensures that we are ready to collaborate and offer top-tier services to our industrial partners.



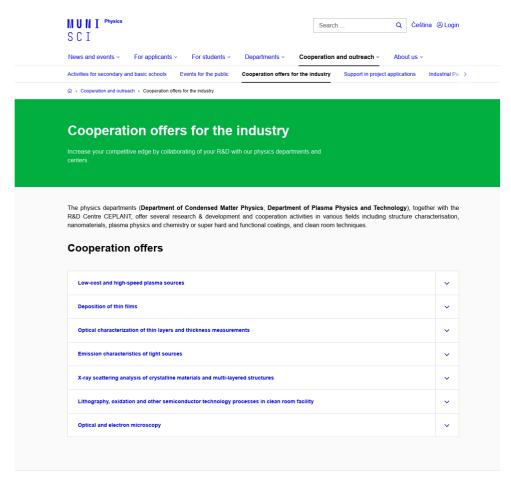
# 3 Examples of Technology Offer Websites of COLOSSE partners

In this section, we provide examples of our websites that detail the advanced technology offerings in materials science, specifically focusing on thin films, coatings, and material characterization. These websites serve as comprehensive resources, showcasing the cutting-edge capabilities provided by Masaryk University, Comenius University, and West Bohemian University.



### 3.1. Example of Masaryk University in Brno websites

Cooperation offers for the industry



#### Are you interested in collaboration? Contact us!

Name (required)	E-mail (required)	
Message (required)		
		SEND

NEWS AND EVENTS News and articles Events calendar

FOR APPLICANTS FOR STUDENTS

Programmes offered Why physics at MU Open Days Study abroad How to apply? Doctoral study

Life in Brno

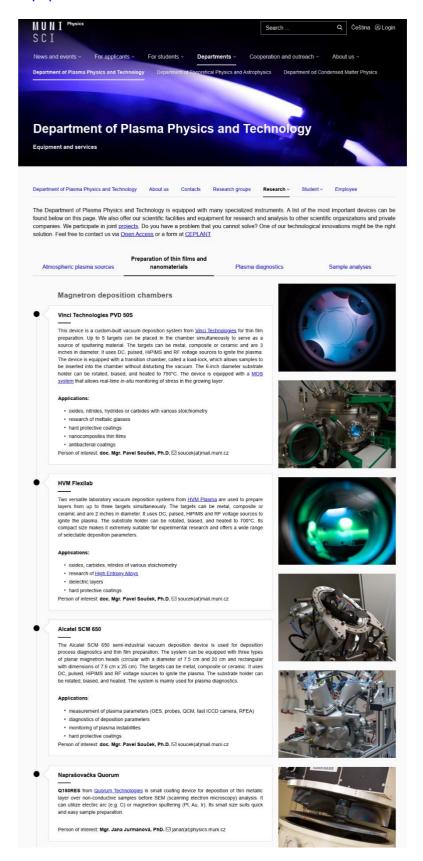
DEPARTMENTS Department of Plasma Physics and Technology Department of Theoretical Physics and Astrophysics

Activities for secondary and About us basic schools <u>basic schools</u>
<u>Departments and R&D</u>
<u>Events for the public</u>
<u>centre</u> Cooperation offers for the Contacts Department od Condensed Matter Physics industry

Industrial Partners



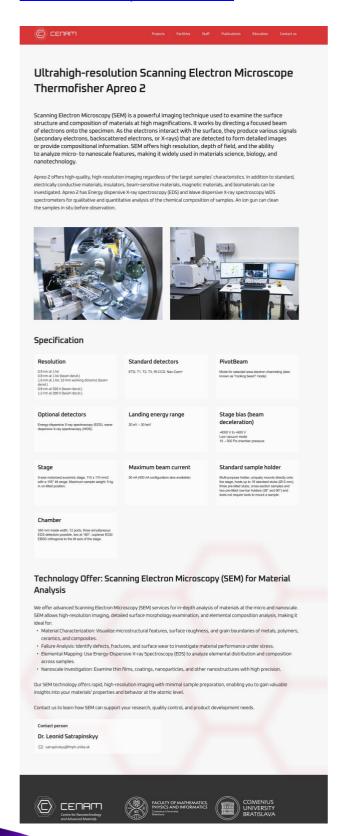
#### **Equipment and services**





# 3.2. Example of Comenius University in Bratislava websites

#### www.cenam.sk/facilities.html



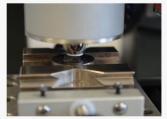




# Nanoindenter Anton Paar NHT2 – analysis of mechanical properties of thin films and coatings

Nanoindentation, or instrumented indentation, is a method used to measure the mechanical properties of materials, especially thin films and coatings. It allows measuring the indenter penetration depth under applied force throughout the loading and unloading test cycle. Data on properties such as hardness [in GPa], astic modulus [in GPa], and creep behavior of materials are calculated from the recorded force-displacement curve.

The Anton Paar NHT2 nanoindentation tester is a robust, automatic instrument for multiple advanced indentation modes: standard nanoindentation, continuous multicycles (CMC), constantmulticycles, progressive multicycles, user-defined sequences, and sinus mode. Unique top-surface referencing for thermal stability, optical microscope, precise positioning, and high throughput enable afast and reliable mechanical surface characterization of metals, ceramics, composites, and even hard polymers.







#### Specification

# Load normal load range: 0.1-90.0.0 mN loading rate: 0.1 mW/min-1.0.0 N/min loading rate: 0.1 mW/min-1.0.0 N/min load resolution: 0.00 ± W frame: stUffness: 107 N/m Standards Sample (ideal sample) filed standards filed standards filed standards Sample (ideal sample) filed standards fi

#### Technology Offer: Nanoindentation Measurement for Material Hardness and Mechanical Properties

We provide cutting-edge nanoindentation services for precise measurement of the mechanical properties of materials at the nanoscale. Nanoindentation enables accurate assessment of hardness, stiffness, elastic modulus, and wear resistance of a wide range of materials, including metals, polymers, ceramics, and coatrins.

hness: preferably a mirror finish; the surface, the more variable the results

Key benefits include:

- High-Resolution Hardness Testing: Measure microhardness with exceptional accuracy, even for thin films or small samples.
- Mechanical Property Profiling: Determine the elastic modulus, creep behavior, and plasticity of materials in localized regions.
- Thin Film and Coating Analysis: Evaluate surface properties of coatings, thin films, and microstructures without the need for extensive sample preparation.
- Depth-Sensing Precision: Characterize hardness and mechanical responses at nano and micro-scale depths for detailed material insight.

Our nanoindentation technology ensures reliable, reproducible data, helping to optimize material performance, quality control, and development processes.

Reach out to discuss how nanoindentation can advance your research and material testing needs.

Contact persor

Dr. Martin Truchlý

truchly@fmph.uniba.s









# 3.3. Example of West Bohemian University in Plzeň websites

New nanostructured thin-film materials

