**Applicant:** Slovak University of Technology in Bratislava

**Project**: Knowledge-based Faculty for Economic Practice

**ITMS code of project**: 26110230113

**Activity**: 3.2

**Responsible for activity:** PhDr. Kvetoslava Rešetová, PhD.

# ADVANCED TECHNOLOGIES RESEARCH INSTITUTE - PROFILE PRESENTATION

| | |
|---|---|
| **Name of activity** | **Activity 3.2** Building the tools for knowledge transfer into education |
| **Specific objective** | **3. Building the tools for knowledge transfer into education** |
| **Aim of activity** | The activity of building the tools for knowledge transfer into education concludes the information flow attained from the analysis of environment impact, and sets up specific tools for the knowledge transfer into education. It is aimed at building a set of tools for transferring the knowledge collected in the previous activities into education at the Faculty, thus enhancing the knowledge base of the target group, while focusing on the functionality of the knowledge transfer to the target group. |
| **Date of activity implementation** | 10/2013 – 09/2015 |

**Project part: activity 3.2 : 1. Tool for knowledge transfer – profile research presentations**

The Faculty research is oriented particularly on the following fields:

- research in materials with focus on the research, development and technological processing of the main types of engineering materials,
- research and development of new technologies in industrial production oriented mainly on technological processing of modern technical materials and environment-friendly production,
- research in identification, automation and control of processes as well as information security of the technology, production and organizational systems,
- research and verification of principles of managerial control and its organizational structures,
- research in quality and certification of processes and products,
- research in safety and reliability of technological devices and systems with emphasis on the methods of systems analysis and synthesis.

The defined research characteristics reflect the Faculty research fields, and are subject to the Faculty evaluation processes. **The current profile presentations comprise the research profile, its identification and recording in a new way**. The Faculty experts in the research fields make the audience familiar with the research characteristics, research and development orientation, so that to provide a comprehensive research profile of the Faculty institutes (there are six institutes at the Faculty) in both Slovak and English languages. The elaboration of text in an adequate number of quires, text translation and copyright rules – all this is subject to the method of the profile presentation implementation. The elaborated profile presentations might be an important material source for:

- training at the Faculty in its key subjects
- domestic and international presentation of the Institute
- enhancement of the advertising space for promotion purposes of the project
- innovative elaboration of the Faculty research contents.

**Defined project outcomes:**

The project outcomes will be determined by successful implementation of the project activities, particularly activity 1.1 - stakeholding, activity 2.1 - portal of companies, activity 3.1 - implementation from acquired e-sources. Such interaction along with the information flow can influence the success of knowledge transfer into education. The outcomes of previous activities will be utilized in this final activity which should provide space particularly for knowledge transfer and improvement of knowledge base, and simultaneously provide a space for meeting the main project aim. Specific outcomes of the activity will be as follows:

- **six profile presentations mapping the research character of six Faculty institutes, applicable in training and with strong potential for the Faculty promotion**
- production of minimum 30 virtual records of technological procedures outsourced from economic practice and applicable in education, i.e. enhancement of information on applicability for the Faculty doctoral students
- production of minimum 30 virtual records of the Faculty technological procedures and processes, for application in the Faculty education, and for the purposes of comparison of the technological processes and theoretical knowledge acquired in the Faculty training to the knowledge acquired in practice
- four expert lectures for doctoral students (and also for interested Faculty researchers), forming the knowledge base of the target group in four principle science fields.

**Implementation of activity:**

1. In compliance with the project aims, the activity was introduced to the Heads of the STU MTF Institutes: **Appendix 1**: Information for institutes of 12 Dec 2013 , **Appendix 2** : Letter to the Heads of the STU MTF Institutes of 21 Jan 2014
2. Heads of the STU MTF Institutes delegated in writing an Institute representative who will be in charge of the profile presentation elaboration – letters to Heads of the Institutes are in the project archive of the principle investigator
3. Individual meetings of the principle investigator with related employees with focus on structure and contents of profile presentations
4. Collection of data, text modifications, graphical design of presentations
5. Text translation
6. Final arrangement of presentations into e-proceedings of scientific papers
7. Publicizing the profile presentations

**Guarantors of profile presentations:**

Institute of Materials – Mgr. Marián Palcut, PhD.

Institute of Production Technologies – Assoc. Prof. Ing. Erika Hodúlová, PhD.

Institute of Industrial Engineering and Management – Assoc. Prof. Ing. Helena Makýšová, PhD.

Institute of Safety, Environment and Quality – Prof. Ing. Maroš Soldán, PhD.

Institute of Applied Informatics, Automation and Mechatronics – Prof. Ing. Pavol Tanuška, PhD.

Advanced Technologies Research Institute – Assoc. Prof. Ing. Maximilián Strémy, PhD.

**Introduction**

The orientation of the STU MTF research activities fastens on the Faculty education profile and is in compliance with the long-term development of the Slovak University of Technology in Bratislava, covering the whole spectrum of the education at STU MTF. The activities of STU MTF researchers are implemented within the following projects:

- projects of base research supported by VEGA grant agency,
- projects of applied research supported by KEGA grant agency,
- projects investigated within international programmes,
- projects of international scientific and technical cooperation,
- projects of base and applied research supported by APVV grant agency,
- contractual research and development (business contracts).

## 1. Science and Research in STU MTF

**Vision of STU MTF**

The STU Faculty of Materials Science and Technology in Trnava, in compliance with the STU vision, intends to be a research oriented and internationally renowned faculty within the similar faculties framework, i.e. the faculties developing modern trends in research and industrial production with focus on progressive materials, sophisticated production technologies and industrial management, automation and IT implementation of production and technological processes such as quality, safety, as well as environmental and managerial aspects of industrial production.

**Mission of STU MTF**

In compliance with the defined mission of the Slovak University of Technology, the STU Faculty of Materials Science and Technology intends to actively contribute to meeting the requirements of the mission – with the priority laid on materials science and production technologies – in accredited fields of education, research and development within the stipulated competences:

- provide the university system of education in all stages in accredited study programmes
- disseminate, improve and develop knowledge by the research and development tools,
- ensure transfer of research results into educational process,
- ensure transfer of research results into entrepreneurial practice,
- protect its research results,
- integrate into the system of university life -long learning,
- participate in sustainable development of society with all its activities, mainly by the development of the student personality in the context of humanism and democracy ideals.

**General and strategic goals of research**

1. Publish the research and creativity results internationally, particularly in the renowned international scientific journals.
2. Increase the STU MTF status in the projects of international cooperation.
3. Build the research infrastructure (equipment) including the qualified service.
4. Intensify the cooperation with practice, ranging from private industrial companies to public institutions and authorities.
5. Focus the research results and free investigation also on the outcomes, e.g. patents.
6. Improve the orientation on other than grant sources from the state budget, particularly on the sources from abroad, project grant agencies and entrepreneurial activity.

**The scientific and research activity of STU MTF is carried out in the forms of:**

- projects of the base and applied research and development,
- projects solved within the international programmes,
- projects of the international scientific collaboration,
- projects of contractual research.

The research content is focused on the following areas:

- materials research with a focus on the research, development and technological processing of the basic and advanced types of technical materials,
- research, development and optimisation of the new technologies of industrial production, oriented particularly on the technological processing of advanced technical materials and ecologically clean processes and products, and the numerical simulation of technological processes,
- process identification, automation and control, as well as information support for technological, production and organisation systems,
- research and verification of the managerial control principles and their organisation structures,
- quality control and certification of processes and products,
- safety and reliability of technological equipment and systems, while emphasising the methods of system analysis and synthesis.

## 1. Profile lecture of the Advanced Technologies Research Institute

### 2.1 History of the Institute

The Advanced Technologies Research Institute is the youngest institute of the STU Faculty of Materials Science and Technology in Trnava. It was established within the University Scientific Park in Trnava in 2013 under the original name of the Research Workplace of Progressive Technologies (VPPT). The workplace bears the current name since 2015.

The first activities of the Institute were aimed at providing education programme of the Development of human resources in the research and development for the Workplace of Materials Research USP-CAMBO. In October 2013, 14 researchers and operators were sent to the Helmholtz Zentrum Dresden Rossendorf (Germany) for a two-year training programme aimed at the training of professionals specialising in materials research and elaboration of projects aimed at the ion beams utilisation. During the training programme, they attended professional lectures and on-site training on unique devices, in order to be able to continue the scientific work at the Workplace of Materials Research within the Slovakion USP.

### 2.2 Description of the Institute

The newly built Advanced Technologies Research Institute (ATRI) specializes in materials engineering in the field of ion and plasma technology, automation, information and communication technologies, as well as in chemistry, physics and astrophysics research, or generally the research into nanotechnologies and nanostructures, sensors, specific hardware and software development, bioengineering and health, computer vision and image processing, big data, humanoids, simulation and modelling. The Institute is the primary user of the facilities and technologies of the University Scientific Park CAMBO in Trnava, built from the structural funds in the total amount of € 42 million.

Ambition of the Institute is to enter as soon as possible the international network of unique research facilities and the recognized research centres in the area. Internationally integrated cutting-edge research will be the basis of the applied research and transfer of new technologies into the industry. In close cooperation mainly with regional industry, the Institute has the ambition to start the activities supporting the introduction of innovations into practice.

The first steps to meeting the above-mentioned objective are the international research projects. From this aspect, the Institute can be considered as successful: for the first year of its existence, it has participated in several international project proposals, and, as a coordinator, won the EU funding for the first phase of the "SlovakION – the Slovak Centre of Excellence in Ion Beam and Plasma Technologies for Materials Engineering and Nanotechnology" project within the Teaming - Horizon 2020 call for the period of 2015 - 2016. The Institute has also signed several international contracts, e.g. with Helmholtz Zentrum Dresden Rossendorf, the top research institute in the field of ion technology. The Institute has also been active and successful in the national VEGA and APPV projects.

In addition to university education on the Doctoral degree in the field of its research, the Institute provides professional training for workers from industrial practice with the aim to promote the transfer and innovation in industry in Slovakia, supporting thereby the economic growth of the EU region.

## 2.3 Workplaces of the Institute

Advanced Technologies Research Institute comprises two Science Centres:

- Science Centre of Materials Research
- Science Centre of Automation, Information and Communication Technologies

## 2.4 Science Centre of Materials Research

The Science Centre of Materials Research represents the scientific and research basis for the application of the ion and plasma technologies in the physical and materials engineering and in nanotechnologies. It is equipped with the top technologies for the modification and analysis of the subsurface and thin layers of solid substances by utilising the effect of accelerated ions and plasma.

The Centre of Materials Research comprises:

- Workplace of Ion Accelerators,
- Workplace of Plasma Technologies
- Workplace of Computer Modelling of The Molecule Properties and Interactions
- Workplace of Chemistry, Physics and Astrophysics.

### 2.4.1 Workplace of Ion Accelerator

The Workplace is targeted at the use of accelerated ions for synthesis, modification and analysis of materials. There are two key devices: 6 MV Tandetron – a linear tandem ion accelerator, and a 500 kV ion implanter. Accelerating voltage of Tandetron is from 300 kV, that of the implanter is from 20 kV. They make it possible to accelerate almost all elements, starting from hydrogen up to gold, except for inert gases. The total achievable energy range of accelerated ions of the two devices represents the interval from 10 keV up to 50 MeV. The maximum achievable energy is 12 MeV for hydrogen, 18 MeV for helium and 50 MeV for heavy elements such as gold. Transport of ion beam and the experiments are performed in a high vacuum. 6 MV Tandetron is used for:

- Ion Beam Analysis (IBA)
- Ion Beam Modification of Materials (IBMM)

Currently, there are two workstations installed:

- analytical experimental chamber
- high energy implantation chamber.

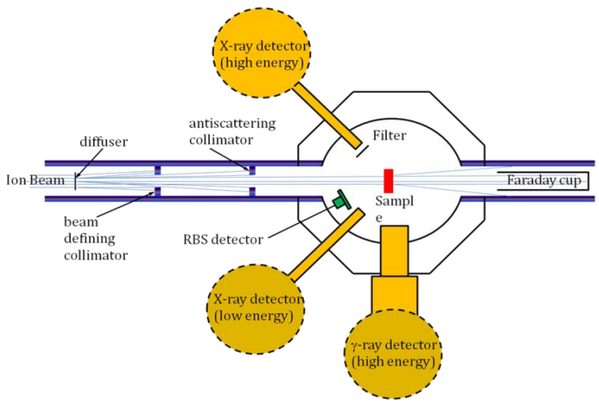
The system is prepared for extension of additional beamlines with endstations and thus for enhancement of experimental and analytical options. System of 500 kV implanter is primary dedicated to ion implantation.

***IBA Workplace***

The IBA analysis by accelerated ions is considered a non-destructive analytical method. High energy ion beam is a very effective tool for the investigation of elemental composition and, to a certain extent, structure of the material surface layers. A focused accelerated ion beam passes through a system of collimators and hits the observed sample. Selection of the detector and arrangement of the experiment depends on the method applied. The interaction of the impinging ions with the atoms of the sample leads to multiple physical phenomena. A typical diameter of the analysing ion beams ranges from 2 mm to 5 mm; a typical beam current is in the order of units and tens of nA. A suitable combination of elements, their energy, incidence angle and the sample material can provide the optimum conditions for the experimental identification of the required information about the sample. Depending on which component of the interaction is detected, the following analytical methods can be considered:

- RBS – Rutherford Backscattering Spectrometry to detect the energy of the backscattered ions
- RBS channelling/blocking – to measure the angle dependence of RBS spectrum of the incident or scattered ions in respect to the crystallographic planes and axis of crystalline sample
    - ERDA – Elastic Recoil Detection Analysis to detect the energy spectrum of the forward recoil scattered ions from the sample material
- PIXE – Proton (Particle) Induced X-ray Emission – to detect the characteristic X-ray energy spectra
- NRA – Nuclear Reaction Analysis – to detect the products of the nuclear reactions induced in the sample by incident ions.

The depth of analysis is typically a micrometer from the surface, in specific cases up to tens of micrometers. It is possible to examine thin layers as well as nanolayers. The surface depth resolution is several nanometers. Analytical sensitivity for the additive elements and impurities achieves the level of ppm.




The essential parts of the PIXE set-up with other related techniques of IBA (PIGE and RBS) .

Fig. IBA

***Brief description of individual methods***

***RBS – Rutherford backscattering spectrometry***

A sample is bombarded by light ions, generally by 1 - 3 MeV helium. It is extremely sensitive to heavy elements in a light substrate. It is a quantitative method without the need of using reference samples. RBS can be used to measure:

- Depth concentration profiles of individual elements present in the sample, including the depth distribution of trace elements,
- Thickness of thin layers,
- Depth composition of the boundary layer structures,

- Thickness of amorphous part on a crystalline substrate,
- Diffusion profile, etc.

It is suitable for the analysis of the elements heavier than oxygen. Sensitivity of the method increases with the increasing atomic mass of the examined elements. RBS in the blocking mode enables to determine parameters of crystalline lattice, quality of crystal, degree of amorphisation, position of additions in the lattice (interstitial, substitutional) etc.

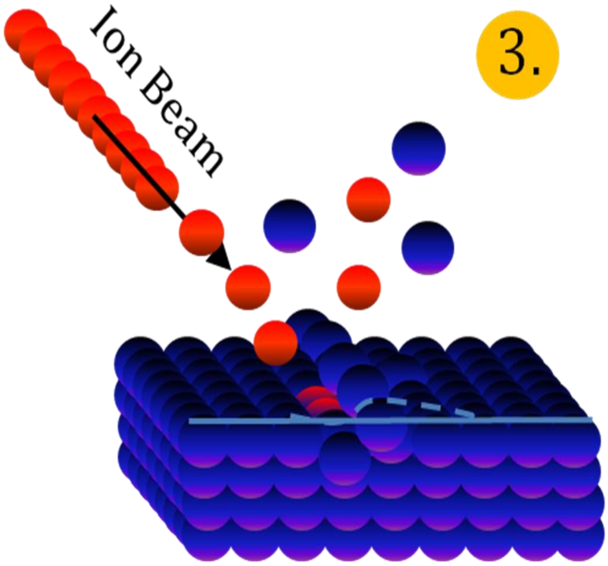
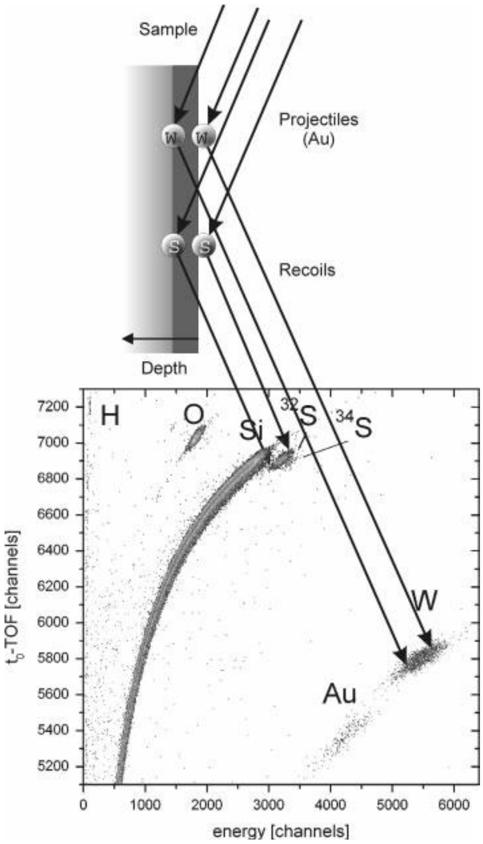



Fig 3 ION

***ERDA – Elastic Recoil Detection Analysis***

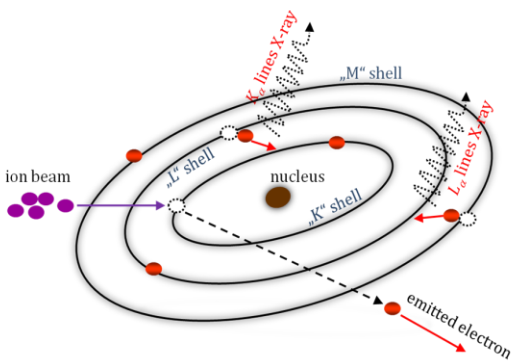
Advantage of the method is high sensitivity to light elements in heavy substrates. The current laboratory equipment enables measuring the depth concentration profiles of hydrogen and light elements. After completing the laboratory equipment, the measuring range will cover also the heavier elements up to uranium.



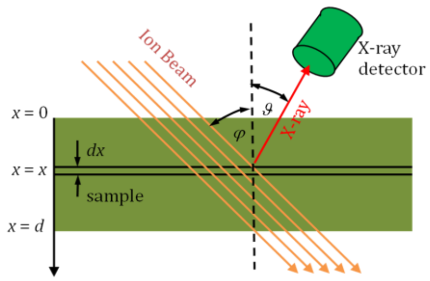

***PIXE – Proton Induced X-ray Emission***

Characteristic X-ray radiation is generally induced by a proton beam of the energy of (2-3) MeV. When interacting with the electron shell of sample atoms, they can be excited, i.e. one of K electrons is rejected from its stable level, or transferred to a higher energy level. Consequently, when the electron returns to the basic atomic energy state, K, L or M X-ray lines that are typical for each of the components may be emitted. After evaluating the detected X-ray spectrum, it is possible to determine the composition of the elements of the atomic number greater than 12 and with the sensitivity up to ppm. PIXE allows the determination of trace amounts of impurity elements in the sample.

One of the most frequent applications of PIXE is monitoring the air pollution or of the liquids contamination, analysis of sediments, geological samples, as well as the artefacts, paintings, archaeological findings etc.




Principle of PIXE: Example of X-ray emission lines in PIXE




Schematic presentation of the PIXE experiment for sample with finite thickness $d$.

***NRA – Nuclear Reaction Analysis***

Measuring parts of the equipment for this method still needs to be completed. NRA uses mainly the resonant nuclear reactions caused by the interaction of the incident ions with the nuclei of the sample atoms. Gamma radiation, as one of the products of nuclear reaction, is the most frequently registered. In addition to the elemental analysis of atoms with low Z, the method enables to measure e.g. hydrogen profile with high depth resolution.

***Simulation of ions interaction with substance***

Within the physical and material research, mathematical modelling and computer simulation are used to prepare, evaluate and interpret the experimental work in the Centre of Materials Research. For this, special computer programs are used to model the processes of ions interaction with the sample material, and subsequently the secondary structural changes in the irradiated material. There are two different approaches to this issue.

• The first approach is based on so-called Binary Collision Approximation - BCA. In this approach, the interaction of ions with substance is considered as a sequence of collisions of pairs of particles. TRIM/SRIM, MARLOWE and other computer programs are used for the purpose.

• The second approach is based on the Classical Dynamics – CD and Molecular Dynamics – MD, when a set of colliding particles is considered as a multi-particle problem. The programs used are e.g. MDRANGE and SIMKIT.

Other programs used in the Institute for simulation and evaluation of the experimental results of measurements are also: RUMP, SIMNRA for RBS, ERDA and NRA, and GUPIX for PIXE.

***Synthesis and modification of materials*** can be implemented via:

- ion implantation
- ion beam mixing

***Ion implantation***

Ion implantation is a process in which substrate is bombarded by accelerated ions. The aim is to incorporate the atoms of additives into the base material of the sample. By changing the energy of implanted ions, the incorporation depth of additive atoms can be modified. By combining multiple energy sources, it is possible to achieve the required depth concentration profile of the implanted element. The ion implantation energy ranges from 20 keV to 50 MeV. The maximum diameter of the implanted substrate is 20 cm for a 500 kV implanter and 10 cm for a 6 MV Tandetron. The substrate can be cooled by water, liquid nitrogen, or heated during implantation.

***Ion beam mixing***

Ion beam mixing means mixing and alloying of atoms in the interface of two different materials by ion irradiation. The method can be used mainly for joining non-equilibrium and metastable alloys and intermetallic compounds.

***Application of ion implantation and ion beam mixing***

The main objective is to modify properties of the surface and subsurface areas of materials. Though implantation is one of the key technologies of the semiconductor industry, it can be also applied to increase the surface wear-resistance, enhance hardness, abrasion-wear, make corrosion-protective layers and biocompatible surfaces. It is also used for targeted modification of the electrical, magnetic, optical and other physical or chemical properties of the surface layers. Another application area is formation of nanostructures and nanoporosity, and modification of their properties.

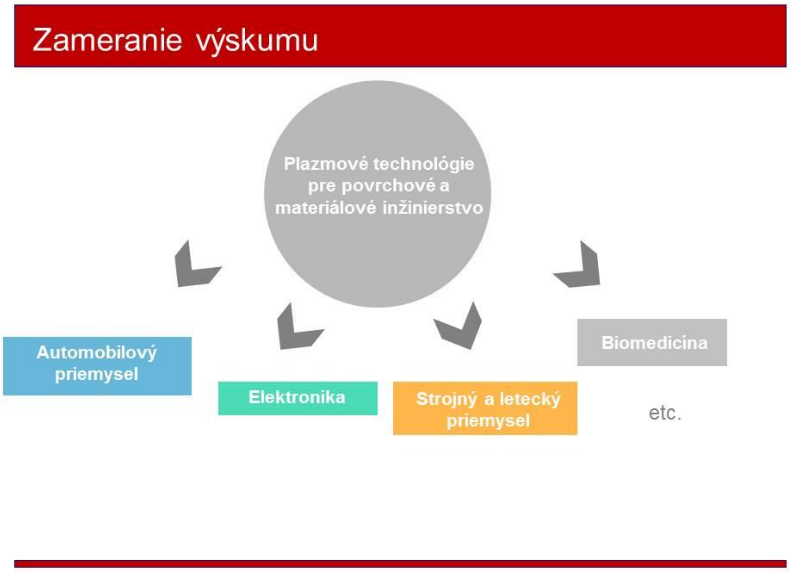
***Further application areas of ion technologies:***

- Exposed parts in the automotive and engineering industries (injectors, camshafts, valves, bearings, etc.);
- Medical and biological applications (prostheses made of materials with originally insufficient abrasion-resistance);
- Surface nitration of stainless steels by ion implantation with the aim to improve their abrasion-resistance while attaining high corrosion-resistance;
- "Stents" (endoluminal blood vessel prostheses), nonporous stents for additionally controlled dosage of drugs, biocompatible and blood-compatible materials, etc., for modern medicine;
- Other options of ion implantation in the areas other than microelectronics, such as the precise mechanics, special construction of expensive watches;
- Protection against high-temperature oxidation (TiAl alloys, turbine constructions);
- Plastics injection into moulds (safety improvement in the removal of parts produced by injecting into the mould, as well as abrasion-protection for highly stressed parts for moulding tools);
- Ion implantation of surface of certain polymers to improve the surface properties, such as electrical conductivity, biocompatibility, etc.

### 2.4.2 Workplace of Plasma Technologies

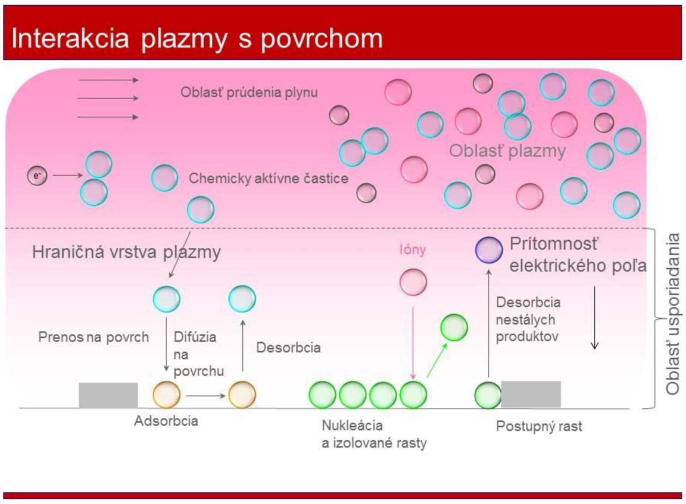
The Workplace research is oriented on:

- *Automotive industry:* Tribology coatings for car engines and surface treatment of components in order to attain higher efficiency and lower environmental load.
- *Electronics:* Transparent conductive layers with improved optical and electric properties.
- *Machine and aviation industry:* Surfaces with enhanced wear resistance and thermal **s**tability.
- *Biomedicine:* Implants with higher degree of biocompatibility.




**Interaction of plasma with surface**

The Figure ???? shows the basic processes in the volume at the interface of plasma and surface of the sample. Ionized particles are produced mainly in the collision of electrons with neutral particles. Active particles are generated by dissociation of molecules that is due to the collision with electrons, or when excited into higher states. The particles are accelerated by the electric field towards the substrate. The electric field generated owing to the different potentials of plasma and the sample affects only the charged particles (ions). The energy of ions then decides about the following deposition, etching or sputtering.

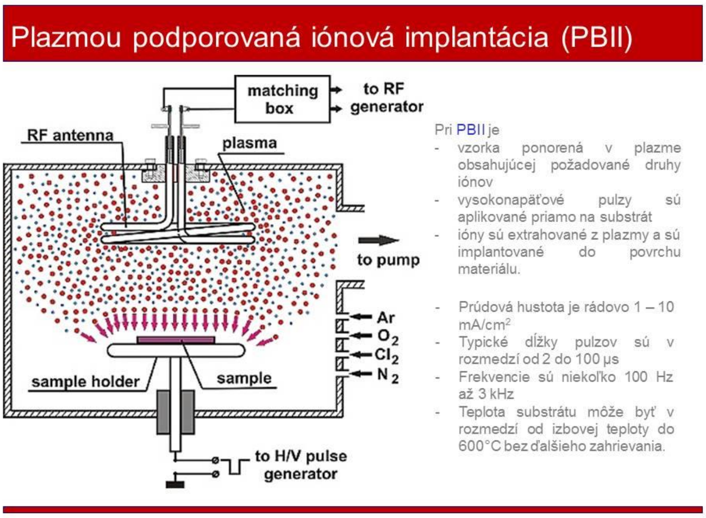


**Plasma-Based Ion Implantation (PBII)**

PBII technique has been developed so as to achieve higher ion current density, in order to substantially shorten the implantation time, as well as to implant surfaces of complex shapes, which is impossible in case of the ion-beam implantation. In comparison with the standard implantation processes, PBII efficiency is higher especially in the case of low-energy high-dose implantation.

During PBII, the sample is immersed in the plasma containing the desired types of ions, where the high voltage pulses are applied directly to the substrate. The ions are extracted from the plasma implanted into the surface of the material.

Current density on the ion beam depends on the plasma parameters and the bias voltage; its value is of the order (1-10) mA/cm$^2$. High voltage in the pulse mode is used to reduce the substrate temperature and to control charging. Typical pulse duration is in the range from 2 to 100 µs at the frequency of several 100 Hz up to 3 kHz. The substrate temperature can be controlled by changing the implantation parameters; it can range from the room temperature to 600 ° C without further heating. Self-regulatory control of charging, achieved by alternating attracting the ions and electrons, allows machining both conductive materials and insulators.

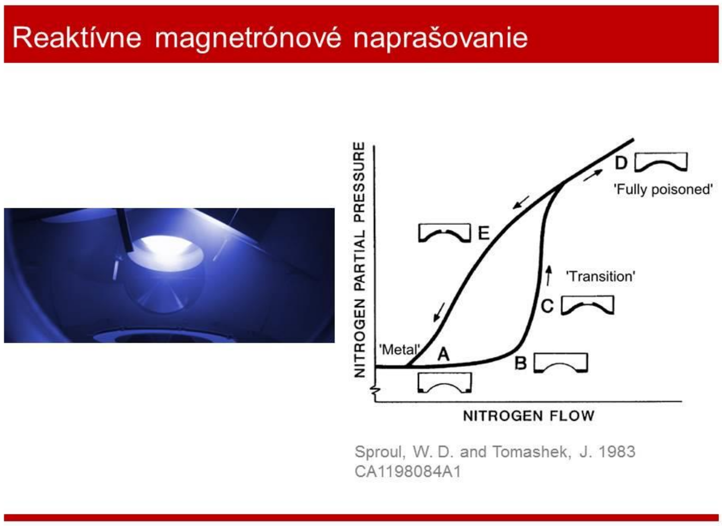



**Application of plasma-immersion ion implantation**

- Doping of silicon by phosphorus and boron by means of the PBII methods for photovoltaic cells
- Super hard surfaces: nitride layers of boron and titanium
- Surface protection of titanium and TiAl alloys: TiAl protection from high-temperature oxidation and progressive coatings for Ti and TiAl alloys
- Biomaterials: nonporous metal materials, tribology protective coatings, antibacterial surfaces, biocompatible surfaces and barrier layers
- Nitration of stainless steel and aluminium

**Reactive magnetron sputtering**

Reactive magnetron sputtering is a popular and proven technology for the production of thin films and coatings such as oxides, nitrides and carbides. In the process of plasma deposition, ions of argon from plasma discharge are accelerated towards the metal target. Incidence of ions on target causes a series of collisions between the atoms of target, which leads to the removal of the atoms. The process of the ion removal is known as sputtering. In reactive deposition mode, a small amount of reactive gases such as oxygen or nitrogen may be added to the process. These react with the material being sputtered to form the desired layer of compounds on the substrate. This may lead to the unwanted effect of the target poisoning. Once the reactive gas is introduced into the process chamber, it reacts with the surfaces, such as walls of the chamber and sputtered target. Intensive erosion (caused by sputtering) in the magnetron channel delays the complete poisoning (forming the mixture) of the channel surface. Poisoning of the channel therefore usually undergoes various stages such as the function of the reactive gas partial pressure and time. The initial phase is the clean metal channel of the target (mode of "metal" sputtering), and the final stage is a completely reacted channel surface (mode of "mixture" or completely poisoned sputtering). Sub-stages are called transition areas.




**Examples of reactively sputtered surfaces:**

(a) and (b) equipment with OLED screen,

(c) anti-reflex layers,

(d) elements of laser optics,

(e) ITO-covered glass,

(f) ITO-covered polymer films,

(g) decorative oxide layers,

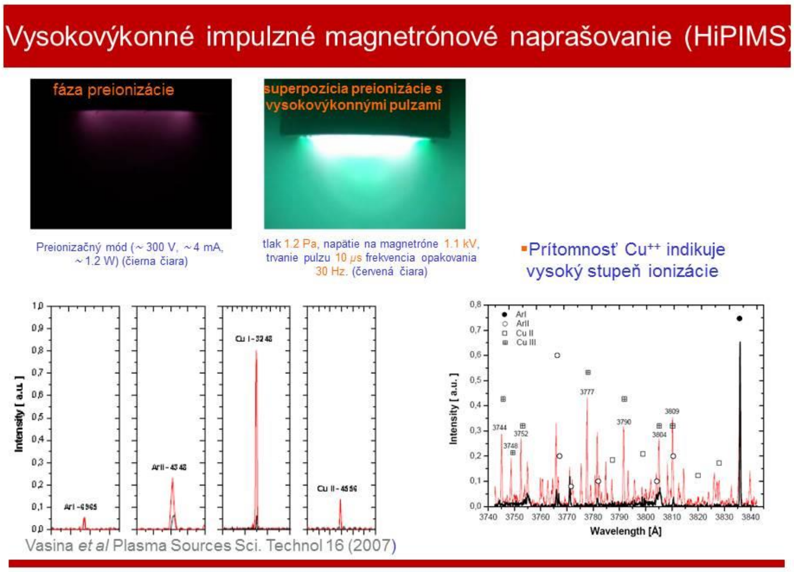
(h) screw taps covered by TiN layer,

(i) milling tools covered by DLC layer,

(j) heat solar panel covered by Ti-O-N layer.

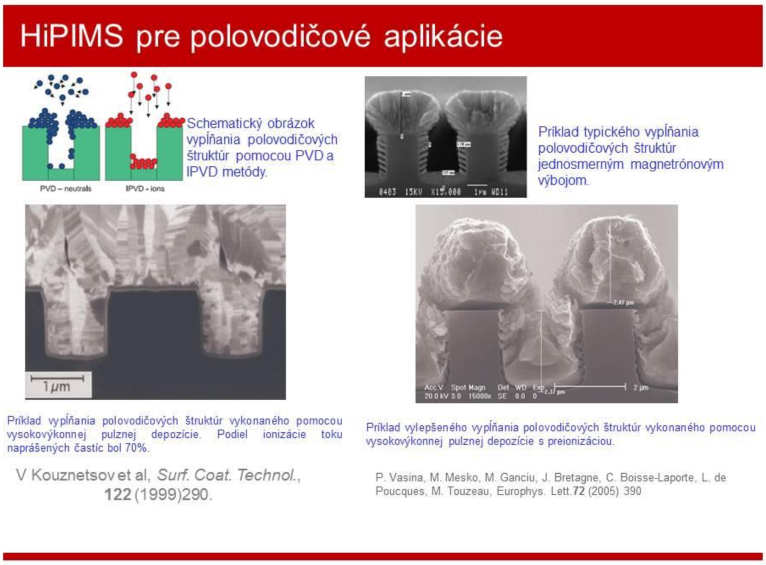

**High-Performance Impulse Magnetron Sputtering (HiPIMS)**

Compared to the DC magnetron sputtering, the energy in HiPIMS is concentrated in short pulses in order to achieve high plasma density, and thus high ion currents towards the substrate. The degree of ionization of sputtered ions is very high, reaching up to 70%.



**HiPIMS for applications in semiconductors**

- Example of a typical filling of semiconductor structures by direct magnetron discharge.
- Example of an improved filling of semiconductor structures by high-performance impulse deposition with pre-ionisation.




### 2.4.3 Workplace of Computational Modelling of the Molecules Properties and Interactions

In accordance with the latest trends, the Centre of Materials Research uses the mathematical and computer modelling to evaluate and interpret experimental work. The used computer programs and approaches are explained in Chapter 8 devoted to the workplace of ion accelerators. They are focused on modelling the process the ions interaction with the sample material, and the subsequent modelling of secondary structural changes in the irradiated material. Specific programs are also used to model the plasma interaction with surface during the ion implantation, as well as to investigate other issues.

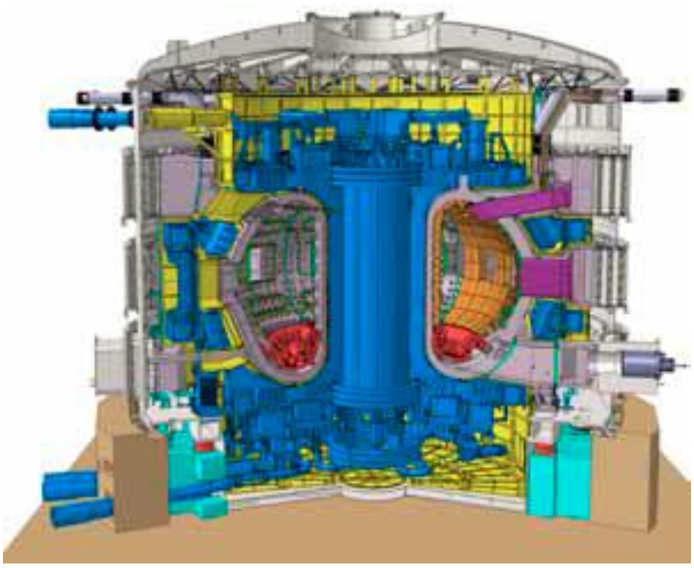
Computer modelling in the workplaces of ion accelerators and plasma technology is focused on direct cooperation within the experiment. The aim of the workplace of computer modelling of molecules and their interactions is the explanation of the elementary steps related to the ion and plasma technologies, i.e. the research into the processes at the molecular level, mainly on the basis of knowledge and precise prediction of the electrical, magnetic and optical properties of atoms and molecules, and their correlation with intermolecular interactions. Some of the elaborated and intended research topics are presented in the following sections.

We will use multi-particle “ab initio” methods of quantum chemistry, especially the method of Coupled Clusters, CCSD (T), CASPT2, CI able to provide very accurate data for smaller molecules and the atomic or molecular clusters, as well as the methods based on functional of density (DFT). In both groups, the methods will include relativistic effects for heavier atoms. Currently available computer programs are mainly MOLCAS, GAUSSIAN, COLUMBUS, DIRAC, VASP and others.

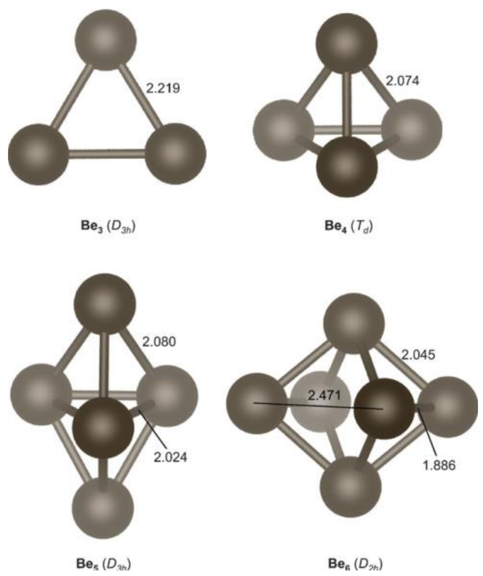
**Non-additivity of interactive interactions in modelling the properties of beryllium**

Metal beryllium is one of the base materials considered for the construction of a fusion reactor walls (plasma-wall material). STU MTF is participating in the research within the EURATOM project. Beryllium is used in alloy steels, in the space research and as an opto-electronic material. In accordance with its electron structure, bonding in $Be_2$ molecule, the smallest molecule component of Be, is extremely weak (van der Waals forces). As a metal, beryllium it is lightweight and hard material. Transition from the molecular properties to clusters of Be and a solid substance is therefore an extremely interesting issue. Working within the EURATOM project, we (J. Šulka, M. Urban, et al., Chem. Phys. Lett. 573, 8-14 (2013)) proved that, owing to multi-particle interactions, the bonding gets extremely stronger even in the small clusters of Be. Pair interactions cannot be used in Be as a starting point, which is very important in modelling Be interactions in mixed complexes with the constituents as BeW, BeH, BeC, BeO etc. that occur as a part of other materials of reactor walls, or as impurities or the particles emitted from high temperature plasma.

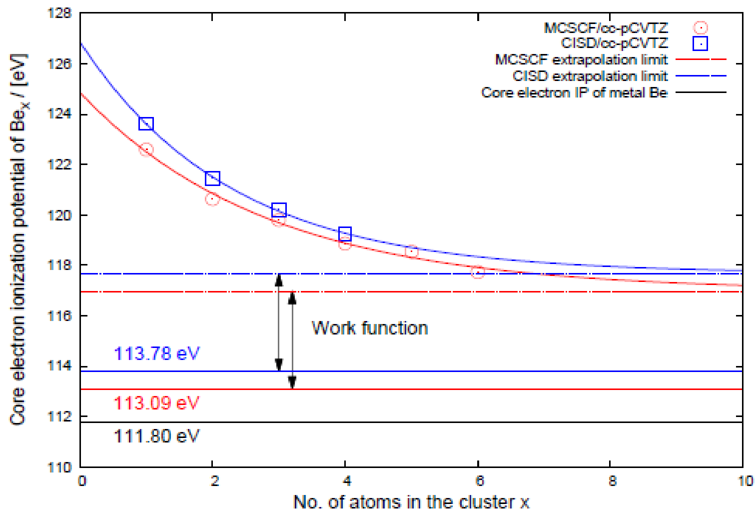
To identify the impurities in the surface layers of Be, XPS method is mainly used. Interpretation of the XPS signal can greatly facilitate theoretical calculations of the inner shell ionization potential (IP) of Be and its clusters. Regarding the multi-particle effects, simple extrapolation of IP from small clusters to macroscopic properties of metal Be is impossible (Fig. 3). Equally important is the understanding of chemical shifts in XPS signal in ionization from 1s orbital of Be, given the bonding in the model compounds of $Be_nH_x$, BeO, BeC, $Be_2C$ etc.



*Scheme 1 of thermonuclear fusion in reactor*




*Scheme 2 Structure of $Be_3$ – $Be_6$ clusters, [M. Šulka, M. Urban and Co., Chem. Phys. Lett. 2013].*




△Figure 4: ΔCASSCF and ΔCISD core ionization energies of Be atom and $Be_x$ (x=2-6) clusters. The IPs show convergent trend with the increasing cluster size. Simple exponential formula of the form $IP(x) = IP_\infty + c_1 exp(c_2 x)$ was used to fit these data and obtain the estimated core electron ionization potential of the cluster of infinite size.

**Fig. 3 Ionisation energies 1*s* for small beryllium clusters. [F. Holka, M. Šulka, M. Urban, Annual Report 2014, EURATOM project]**

**Nano-clusters of mint metals and their interactions with ligands**

Gold nanoparticles are particularly useful as chemical catalysts or growth accelerators of other nanostructures, i.e. the applications in which the size, structure and composition are essential. In addition to their use in catalysis, they are considered for the applications in nanotechnologies, development of advanced materials, optical and nonlinear optical processes in molecular systems, as well as in biology and medicine. Study of the principles of metals interaction with ligands provides the basis for understanding the interaction of metals with proteins on the orbital level that can further serve as a basis for the design of new metalloproteins with programmable properties. The relationship between structure and the activity determined by the properties of nanoparticles is important for their safe application.

In a series of papers, culminating in a detailed analysis of the interaction between the free ions pair of ligand (L) and a coin metal (M) (M. Urban, et al., J. Phys. Chem. A, 117, 4472, (2013) we showed that its driven force is donation from a lone pair combined with the back donation (particularly in the case of the ligands containing the atoms of P and S,).

Based on the molecular data (ionization potential (IP) and electron affinity (EA) of ligands and clusters of gold, it was possible to estimate relative stability of various clusters. We simultaneously tested a series of DFT functionals for their use in larger clusters up to nanostructures, which opens the chance of studying a cluster using DFT with checking the accuracy of based on CC calculations of smaller complexes. Remarkably, EA of $Au_n$ clusters oscillates with their size (Assadollahzadeh B., P. Schwerdtfeger, J. Chem. Phys., 131, 064306, (2009), expressing thus specific features of nanostructures according to their size.

This is also reflected in their interactions with ligands; interaction energies of $Au_n$ clusters with ligands L will similarly oscillate with their size and specific structure. Preliminary results confirming this hypothesis are depicted in Figure 6. We also intend to expand the number of ligands in $Au_n$ clusters to study the $Au_n$ - Lm model in order to formulate general rules for the stability prediction of these clusters, corresponding to their size up to the nanoscale.

In addition to the interaction of free electron pairs, we will also focus on the ligands with an open valence shell (so called SCX3, basic elements in the formation of self-organizing monolayers self-assembled monolayers and SAMS), e.g. $CH_2$ ligand. Also of interest are the optical properties (polarisability in particular) of the Cu-L, L-Ag, Au-L (M-L) clusters. We will test the assumption that, during the M-L interaction, polarizability of the complex increases as a result of the charge transfer, and that this change will be proportional to the strength of "bonding".

It will be interesting to verify whether and how this simple relationship can be influenced by retroactive donations.

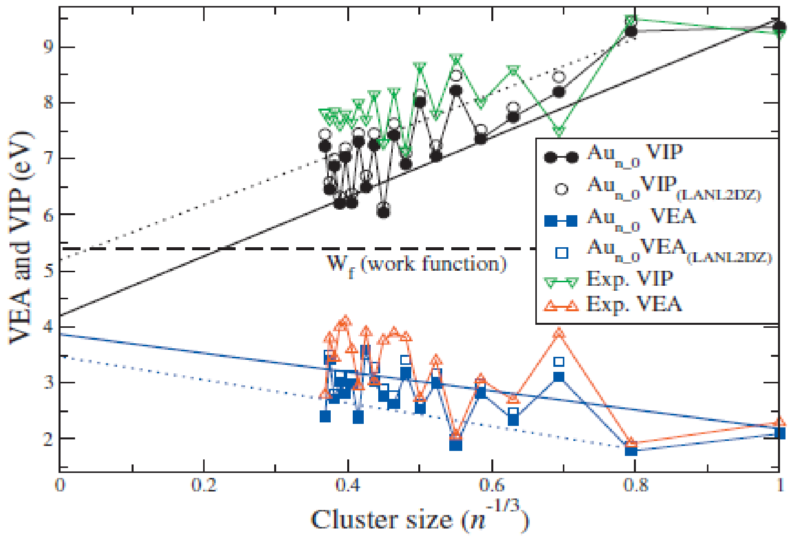



**Fig. 5. Oscillations of electron affinities of ionisation energies of the cluster size $Au_n$**
**[Swerdtfeger and Co. J. Chem. Phys., 131, 064306, 2009]**

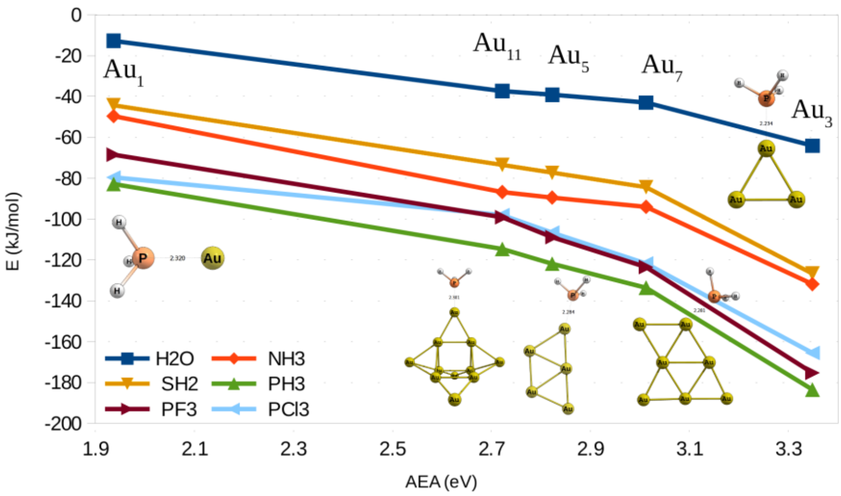



Fig. 6. Interaction energies of ligands with $Au_n$ and their dependence on the electron affinity of $Au_n$ cluster. [M. Urban and Co., Internat. Congress of Quantum Chem. Peking, 2015].

**Confinement - a model for calculating ion polaribility in crystals and other materials**

To understand the interactions on the surfaces of ion crystals, it is essential to know electrical properties of the ions participating in the crystal lattice. These are quite different than those for the isolated ions. Certain ions, such as anion of oxygen $O^{2-}$ is unstable as a free particle, but it stabilizes the external environment, e.g. in the ion crystal.

Changes in the ion polaribility in the environment can be modelled using an external boundary potential, representing the confinement. We intend to expand the calculations of in-crystal polarizabilities of anion to cations in order to recognise the macroscopic properties of glasses and crystals. Ion polaribilities are closely related to the dipole-dipole dispersion coefficients, and hence the van der Waals interactions between the ions. Model of confinement can be applied also to an interesting area of development and understanding of structures such as quantum dots.

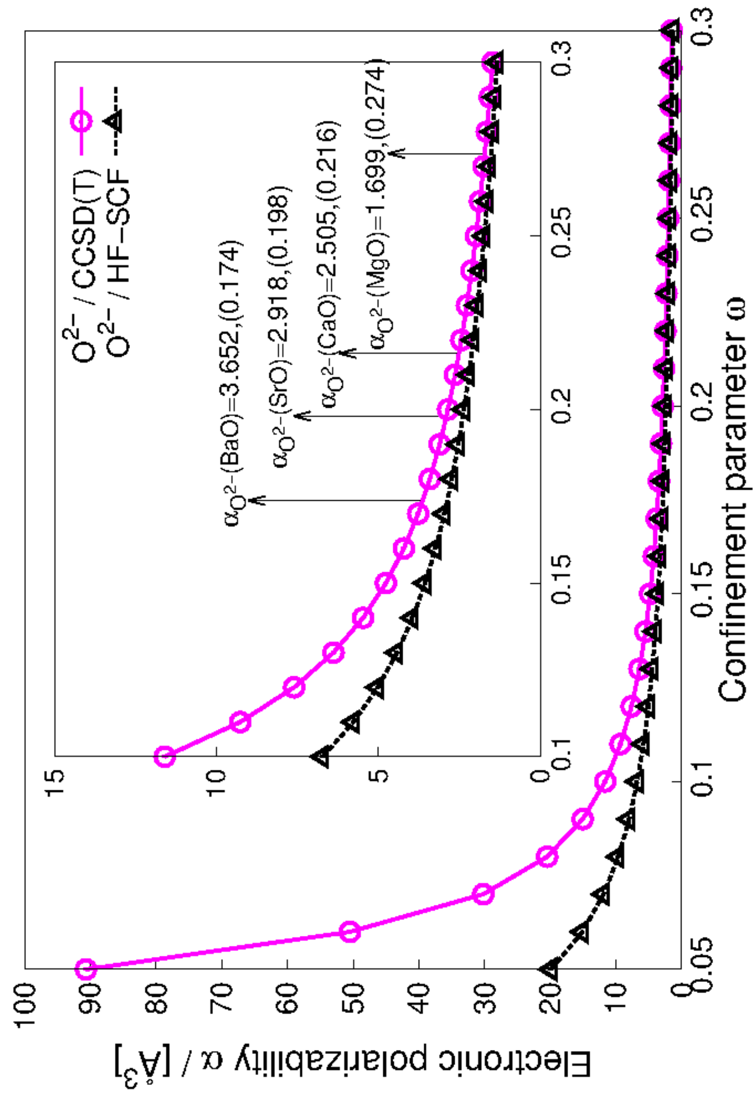



**Fig. 7. Polaribility of $O^{2-}$ anion for various crystals and its dependence on the external confining ω potential [F. Holka, M. Urban, P. Neogrády, J. Paldus, J. Chem. Phys. 141, 214303, 2014].**

**2.4.4 Workplace of Chemistry, Physics and Astrophysics**

Astrophysical research at the Institute focuses primarily on the study of accretion processes in some types of interacting binaries, i.e. pair of stars in which one loses the mass which is then accumulated on the other object which is rather exotic. It is a white dwarf, a neutron star or a black hole. Our concern is the process in which the matter is transferred from one star to another.

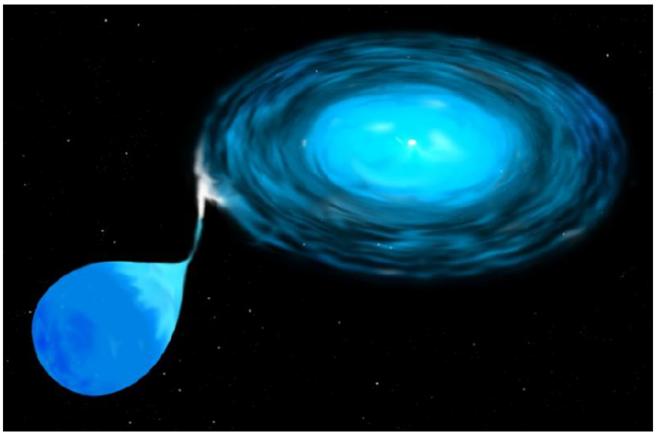
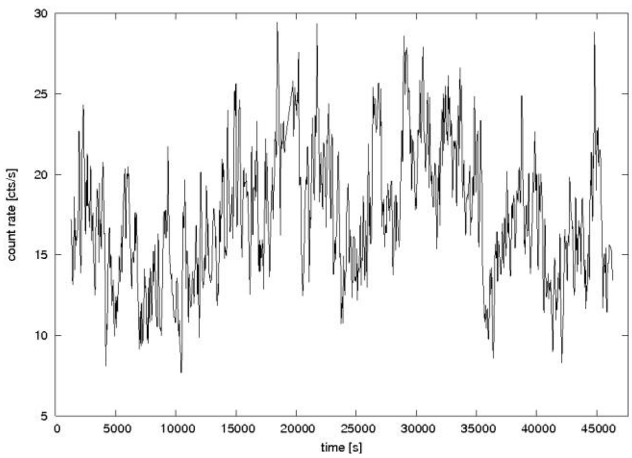


**Fig.** according to: http://commons.wikimedia.org/wiki/File:Accretion_Disk_Binary_System.jpg

So called accretion disk originates in the absence of a strong central magnetic field. It is a source of interesting radiation processes observable on a wide scale of the electromagnetic spectrum. Magnetohydrodynamic processes in it take place in the conditions inimitable in terrestrial laboratories. The mass flow through the disk is unstable and highly turbulent. Many other time-varying factors determine its physical properties, and hence the irradiation. The disc therefore does not emit light constantly, but changes its radiant performance in various time scales. The object of our study is thus a kind of twinkle which seems to be chaotic at first sight.



Radiation intensifies and attenuates completely unpredictably on a time scale of seconds up to tens of minutes. In case of exotic objects with black holes, the changes of clarity can take even less than a second. One possible reason is the above-mentioned unstable and turbulent flow of substance, resulting in the unstable energy generation. Statistical characteristics of the twinkle can therefore bear a lot of information about the hydrodynamic properties of gas or plasma in accretion disks. This chaotic phenomenon is studied in the visible and X-ray regions of the spectrum. We are dealing mainly with computer simulations of this phenomenon and the modelling of light curves, thus trying to find a physical model that best simulates the actual measured data. The best model should describe what is happening in the disk. The actual measured data was analysed either by foreign researches or we use the public or our own satellite observations.

The best data from the visible light were supplied from the Kepler satellite. It is an American NASA probe made for the purpose of continuous monitoring of one area of the sky, searching for the smallest changes in brightness of stars. It is a manifestation of the planets passing in front of its parent star, and covering it partly for a while**.**

***Fig. Photo, Ball Aerospace [***http://kepler.nasa.gov/multimedia/photos/?ImageID=20]

The original purpose of Kepler satellite was the search for so called exoplanets, i.e. the planets circling around the stars other than Sun. Besides, the satellite monitors a lot of other objects in its visual field. This enables us to analyse light curves in the horizon of hundreds of days with a cadence of approximately one minute, which is incomparable with terrestrial observations.

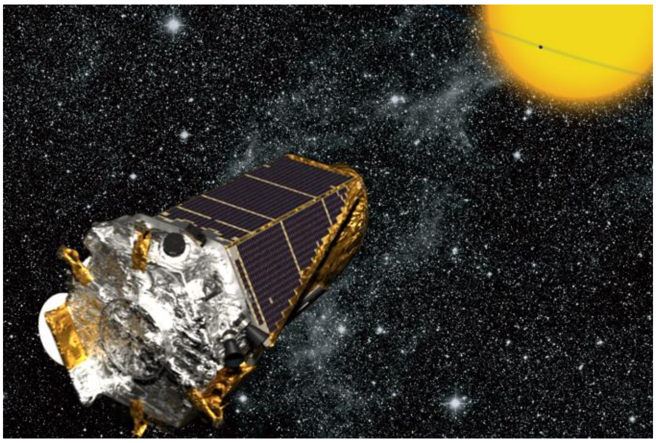


**Fig. Photo, NASA/Kepler mission/Wendy Stenzel.**
**[http://kepler.nasa.gov/multimedia/artwork/artistsconcepts/?ImageID=145]**

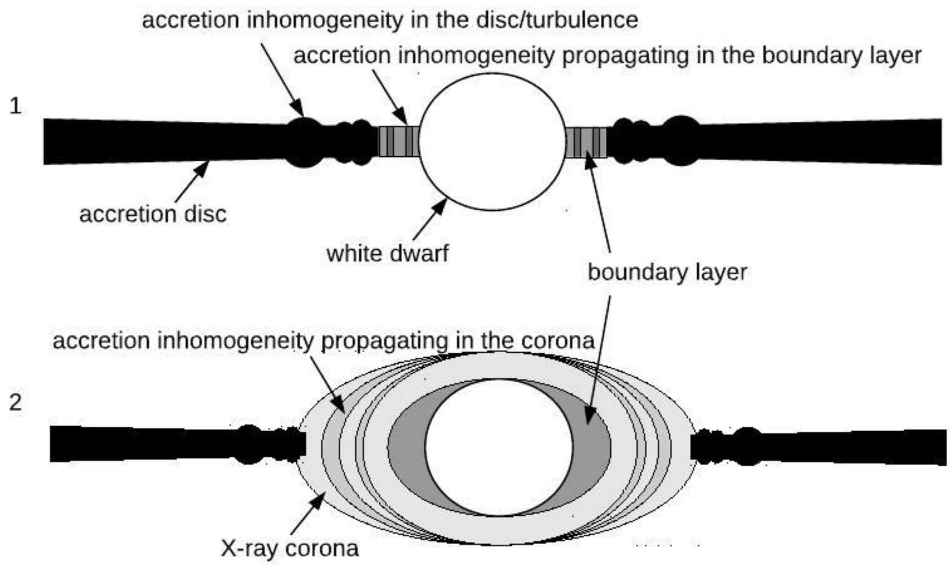
The closer the falling mass to the central star is, the more energy it irradiates. The most intensive radiation is in the X-ray region of the spectrum. Such radiation cannot be observed from the Earth ground, and therefore the instruments on the orbit are used.


**Fig. Photo, ESA/XMM-Newton.**
**[http://xmm.esac.esa.int/external/xmm_science/gallery/public/conditions.shtml]**

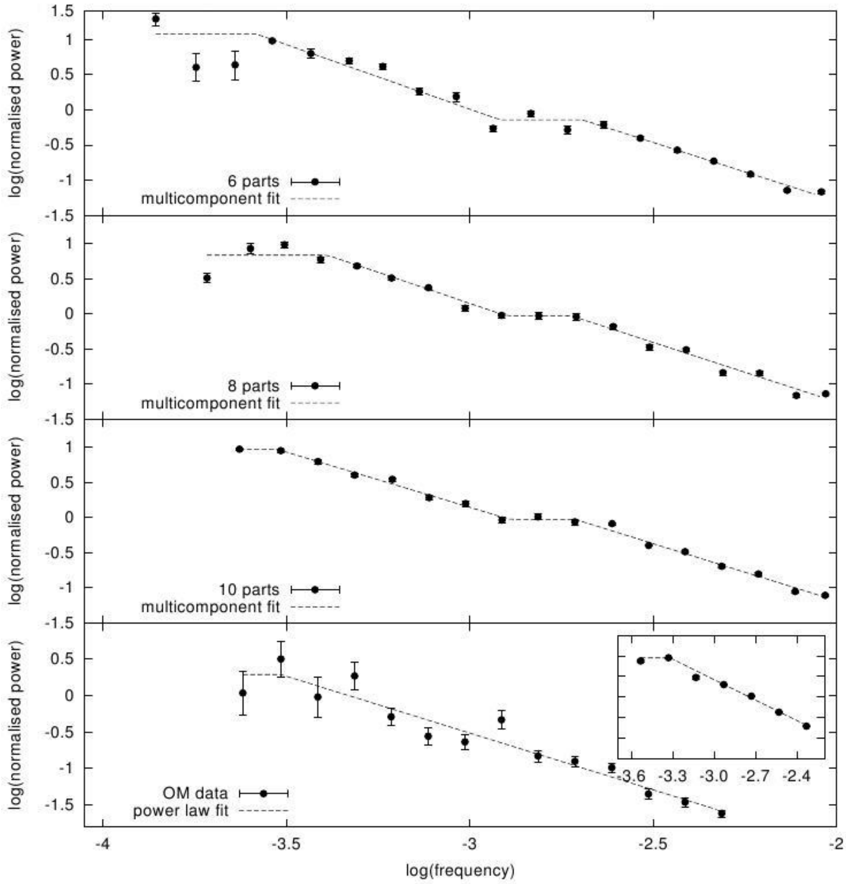
We used the available data of a binary (double-star), and now we are waiting for our own observation time of another double-star system by using the XMM Newton probe launched by the European Space Agency (ESA).

**Fig. Photo, ESA/XMM-Newton.**
**[http://xmm.esac.esa.int/external/xmm_science/gallery/public/conditions.shtml]**

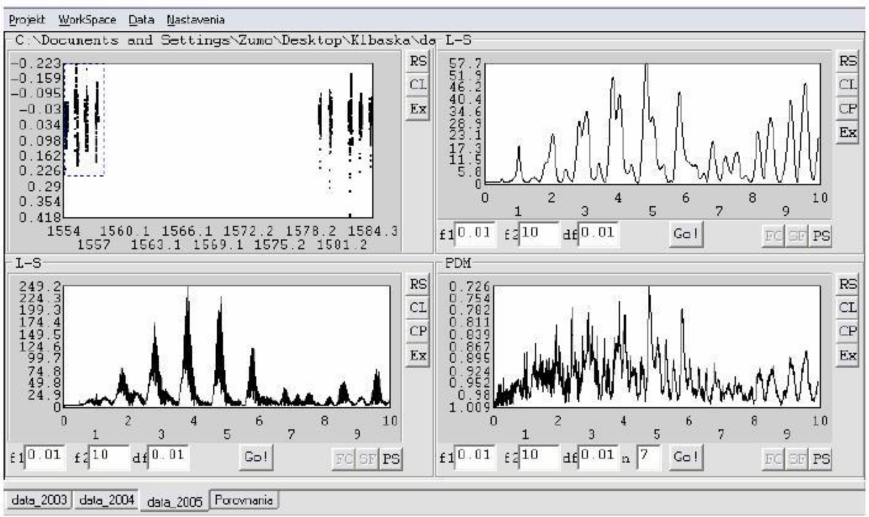
The picture illustrates our effort to get a complex physical model of a mass falling from one star to another, contributing thereby to disseminating the knowledge of the physical processes present.



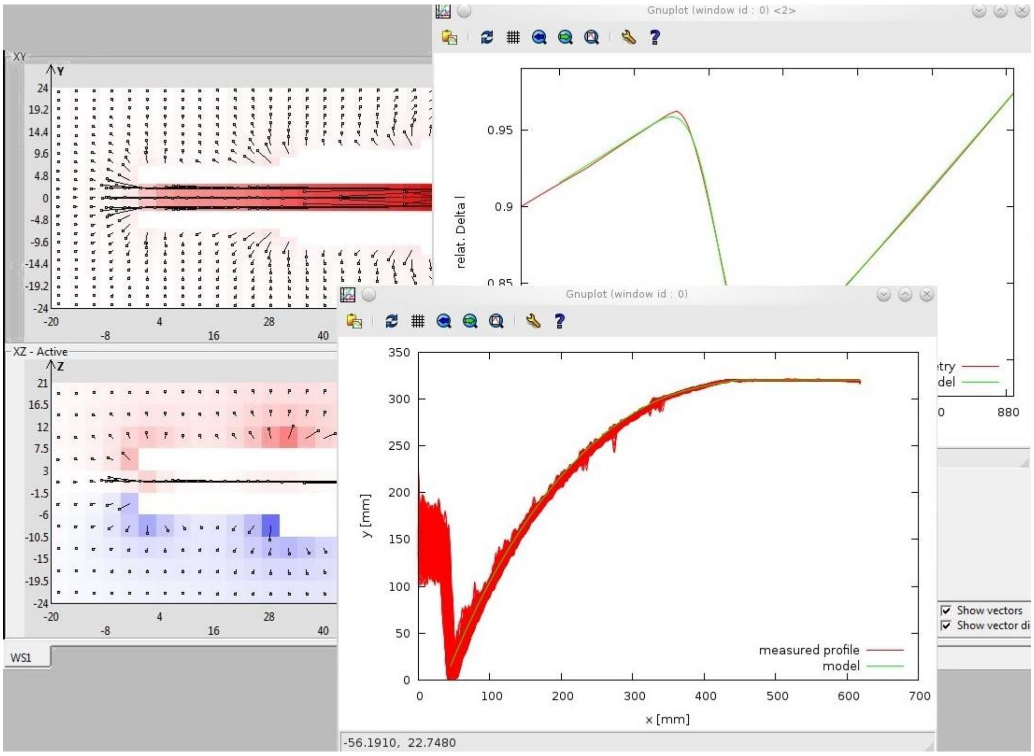

At first sight, our theoretical research seems to be of no obvious practical application. Rapid oscillations generated by the accretion process in the studied binaries exhibit the character of so-called red noise. Thus, the Furrier image in logarithmic scale is a decreasing linear function with increasing frequency. Red noise is typical for the stochastic processes studied in many disciplines other than astronomy both on Earth and in its immediate vicinity.




An example of the application of astronomical studies in other is the development of software for the period analysis of astronomical data. It was originally designed to find coherent periodicities in astronomical observations, but it is ready for general use in any kind of records to study the frequency and structure of records. The anticipated results are the time series, but also the material images from the microscope, that have their own texture and structure. It is not necessary to list other application options, since the Furrier analysis is an individual scientific discipline.



In examining the above-described phenomena, we are developing other original analytical programs. They focus either on the Monte Carlo simulations, or optimization of parameters. This is another example of using these mathematical methods outside the field of astrophysics. In such a way, we deal with many practical tasks such as modelling the magnetic fields around the coils in the electromechanical safety relays, measuring the radii of the rounded components of the bearings used in confocal microscopy, modelling the time course of the tool steels dilatometry, etc. mathematical and statistical apparatus of Our astrophysical research thus contributes to solving the practical tasks.




**2.5 Science Centre of Automation, Information and Communication Technologies**

The Centre focuses on the base and applied research in the following fields:

- Automation and control engineering in industry
- Artificial intelligence, machine learning, human-robot interaction, robotics etc.
- ICT and medicine
- Modelling, simulation and optimisation of production systems
- Big data, business intelligence, data mining, knowledge acquirement
- Mathematical models and representations (systems with fast feedback)
- Computer vision and picture processing
- Microelectronics and hardware development, microchips
- Technology of sensors, pneumatic systems and drives, management and control systems, industrial communication technologies
- Software development (GIS , telemetric systems, distributed control systems), SW verification and testing
- Integration of the information and management control systems
- Bioengineering, medicine / health
- Interdisciplinary technical sciences.

The Centre provides support to other components of the Institute and the Faculty in the fields of industrial automation, data acquisition and processing, electronics, microelectronics and other related areas.

Our equipment allows, inter alia, carrying out the tests using an analogue-digital simulator connectable to the real industrial camera system. The Centre is involved in various domestic and international research projects and preparation of technology proposals of submitted projects, where knowledge of the latest technologies and trends is required. One of the objectives is to acquire our own research projects and raise funds for them from various grants.

The current projects deal with the measurement of residual power of the spent nuclear fuel, or the design of the technology and system solutions for MONES project that is focused on telemetry in the vicinity of nuclear power plants and factories. Within the latter, we have optimised the designed communication protocols for the devices communicating via radio modems.

Besides the participation in industry projects, we also cooperate with experts from the fields of healthcare, safety, monitoring and other technologies.

Our expertise is based on continuous monitoring of the current trends and practical experience in various technology solutions. Examples include practical solutions of a saw for cutting polystyrene or manipulator for the automotive industry with enhanced features such as safe automatic return.

The current trend of Big data and various Cloud-systems enables processing and storing huge amounts of data. This area provides a wide range of research options for the Centre, starting from design through implementation in a real or virtual environment, up to the acquisition and distribution of data from various sensory systems for databases.

***Medical informatics***

In 2014, the Centre started a relatively strong cooperation with the Slovak Medical University in Bratislava in the fields of applying mathematics, modelling, automation of data processing, informatics and related technologies in medicine with the aim to design special equipment for the health care and health monitoring systems. This resulted in the research projects in the fields of environmental pollution, geostatistics and prediction of the development and monitoring of substances in the Slovak Republic citizens, as well as the submission of a proposal within the international project calls of H2020 in the field of neuroplasticity.

Another area of research is artificial intelligence, machine learning, human-machine interaction and robotics.

The voice-operated robot in the video is able to detect, identify and properly grasp the subject, which requires the implementation of the entire spectrum of the machine learning methods and mechatronic systems. This is a multidisciplinary field of the human research, regarding the structure of the kinematic mechanism (53 degrees of freedom in this particular case) or the control algorithms based on artificial intelligence, as well as a number of different touch sensors, voice recognition, and image processing.
We used the results of various disciplines, such as:

- Artificial intelligence
- Computer vision
- Processing the natural language
- Robotics
- Human-machine operation
- Mathematics

- Psychology
- Cognitive science
- Computer neuroscience
- Philosophy of thinking
- Various engineering disciplines
- Software development

Research in robotics and cognitive systems is essential for the progress towards the machines with human abilities. Many innovations have appeared as a by-product of robotic research.

**Features of Cognitive Systems**:
• Artificial cognitive systems are able to perceive, understand and learn from the individual and social interactions with the environment;
• Social objectives are then design and development of scientific foundations of artificial cognitive systems, while learning from the natural cognitive systems;
• Research into artificial cognitive systems is expected to bring new technologies opening the way for various applications involving the interaction with the real world and its people.

In future, it will be necessary to solve various tasks, such as:
- Ability to learn from experience - it allows the cognitive system to adapt to external conditions and their changes;
- Robustness - the ability of robots should not dramatically worsen in case of unexpected events and observations;
- Efficiency - improved performance means the ability of cognitive system to predict, both in the near and distant future;
- Natural behaviour - tolerant to ambiguity and uncertainty arising e.g. from the cooperation with people; abilities of robots should be improved in time.

The current EU and global trends of using intelligent robots in industrial automation will require the deployment of the above-mentioned cognitive systems into the areas of fixed programming of the robot without the interaction with man. All the leading manufacturers of industrial robots have recognised the current trend and are developing the robots with sensors and feedback, enabling safe interaction with humans. It is not the effort to replace the human workforce by robots, but to facilitate the work of the human workers in the production line, while eliminating various repetitive and physically demanding operations. Robots with artificial intelligence will be able to carry out certain activities learnt from humans, based on voice commands. This requires coordination of the above-mentioned robotic sensors, actuators, drives and cognitive systems. Baxter robot is an example of a robot deployed in industrial automation in North America. It is safe and flexible, carrying out the tasks such as loading and operating machines, packaging and handling materials. It requires no manual programming, learning instead, and thus reducing the time and cost of programmers.

The video shows the robot performing repetitive tasks, while man just supplies the required components to certain places, without the need of strict compliance with the specific location; the robot is able to detect the location of parts, and the robot system will enable to grip them correctly.

Since robotic grasping is still a big problem, there are many scientific approaches to improving it. One of them is the method of so called deep neural networks, i.e. neural networks with multiple hidden layers. It allows us to elegantly solve the issue of machine learning, which was until recently almost unsolvable or very time-consuming. It is due to the ever increasing power of computer graphic processors. Why graphic when it concerns a robot? Architecture of modern graphics processors is based on a large number of discrete graphics units, up to a few thousands in a single processor, which, when compared to computer chips, provides much greater performance and are perfectly usable in simulations of neural networks, requiring a high amount of simulated neurons and individual layers of neural network. The technology of deep neural networks falls within the so-called **Deep Learning**. This approach includes also so called convolution neural networks.

***Convolution neuron nets***

Recognition falls to several levels. Each level represents a certain degree of abstraction of the input pattern. From the levels that detect single local symptoms, to the levels that recognize the whole objects in the submitted patterns. The principle can be used in conventional feedforward multilayer networks. The networks of this type will have many hidden layers, which will allow hierarchically decomposition of the problem into several parts, and thus accelerate the learning process. The method for deep network learning was designed in the year 2006. The designed deep network (called Deep Belief Network) consists of the layers of Restricted Boltzmann Machine (RBM). The version of deep network designed later consists of the layers of autoencoders. Both deep networks succeeded in learning, mainly thanks to pre-training without a teacher.

***Modelling and simulation***

Applied research in the field of **simulation** and **modelling** is implemented by means of the Witness and Plant Simulation tools. The tools serve for the simulation, visualisation, analysis and optimisation of the production and logistic processes.

Simulation is a research method, where an examined dynamic system is replaced by its simulator that is then used for experiments with the aim of gathering information about the original examined system. It is so called computer simulation, where simulator is created by a debugged simulation program.

Simulation is widely used as a support tool of decision-making in the management of the existing or design of the new production systems, e.g. in automotive industry, supply chains for the automotive industry, logistics, aviation, shipping industry and services.

Main roles and advantages of simulation are:

- Decision-making support in designing a system and in its operation
- Analysis and optimisation
- 2D or 3D visualisation
- Predicting and "foreview"
    - Replacement of a real system (possibilities of training and testing, while avoiding dangerous situations and cost of eliminating the consequences etc.)

Simulation study is implementation in four stages:
1. Analysis of the current state
2. Making a simulation model
3. Design of experiments
4. Recommendations based on the results.

The entire process of simulation project involves the system analysis, problem definition and formulation of the simulation objectives, collection and processing of the information from the process, estimates of parameters and types of distribution of random quantities; building an abstract logical model; construction of the model in computer; verification and testing of the model – verification and validation; planning and preparation of simulation experiments; implementation of simulation experiments (changes of factors in the model), or modifications of the model. This is followed by the evaluation and processing of the experimentation results, elaboration of the final report and recommendations.

Principle of simulation is simple. Instead of observing the course (dynamics) of a real process, we observe behaviour of a simulation model of the given process.  Such approach brings a lot of advantages by enabling the:

- Examination of  behaviour of non-existing so far (designed) systems,
- Comparison of behaviour of various versions of the system – regarding the selection of production devices,
- Options of their space arrangement and management algorithms,
- Assessment of the production options of various product assortments,
- Verification of the system behaviour in a relatively short time and a long-term horizon.