

The Czech Academy of Sciences

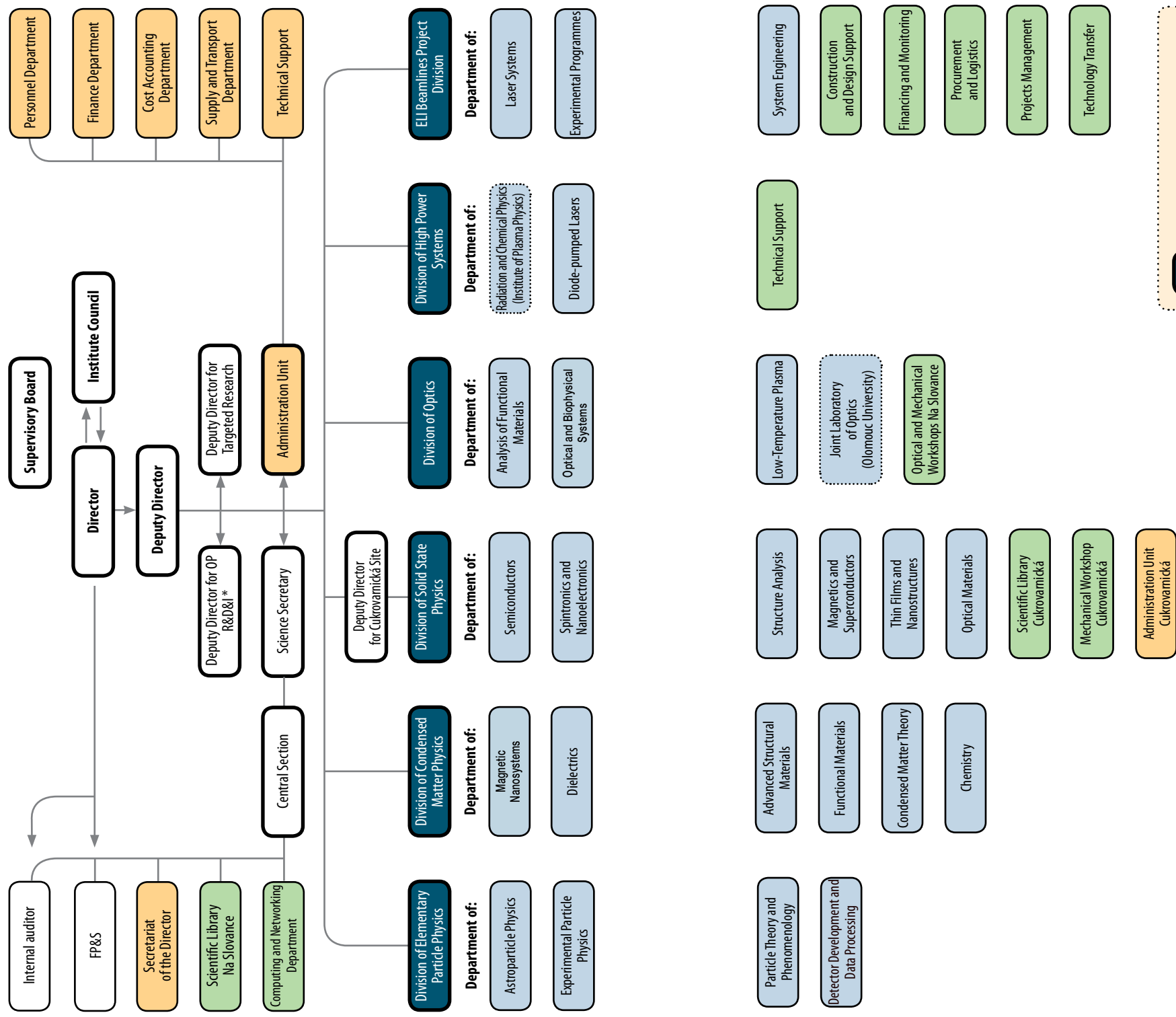
Institute of Physics



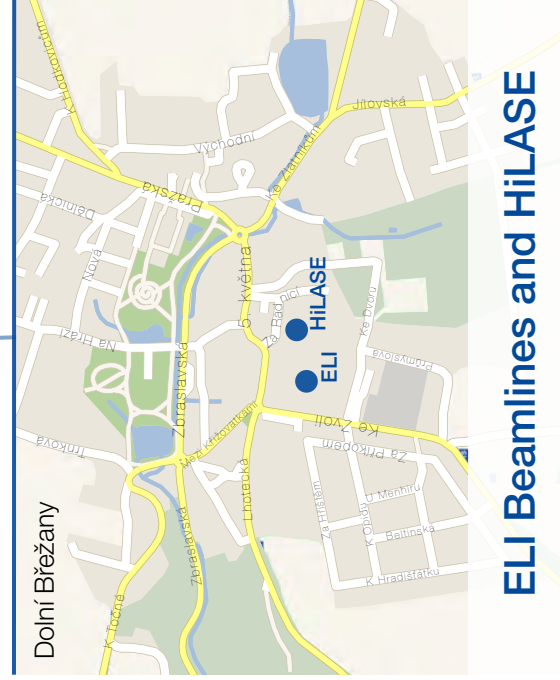
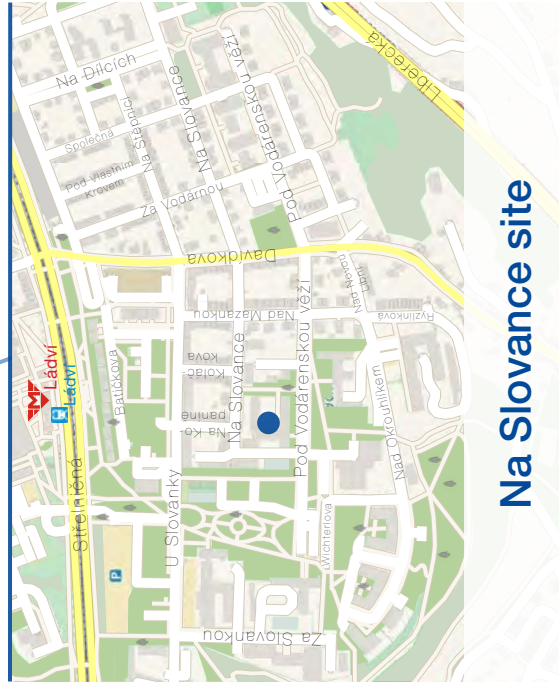
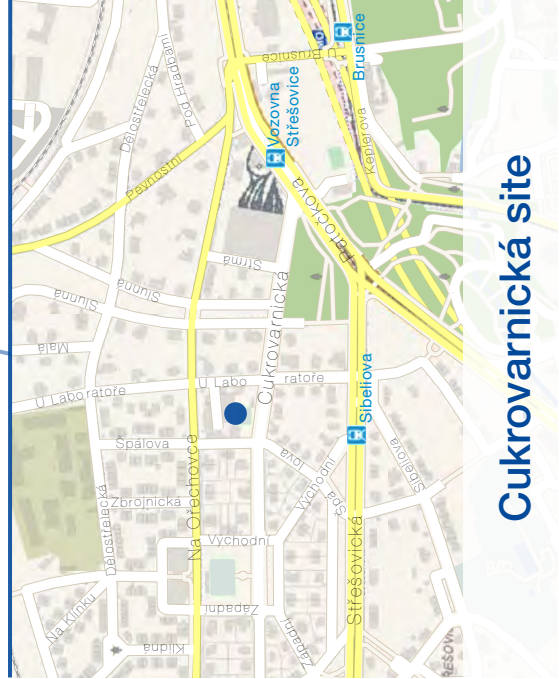
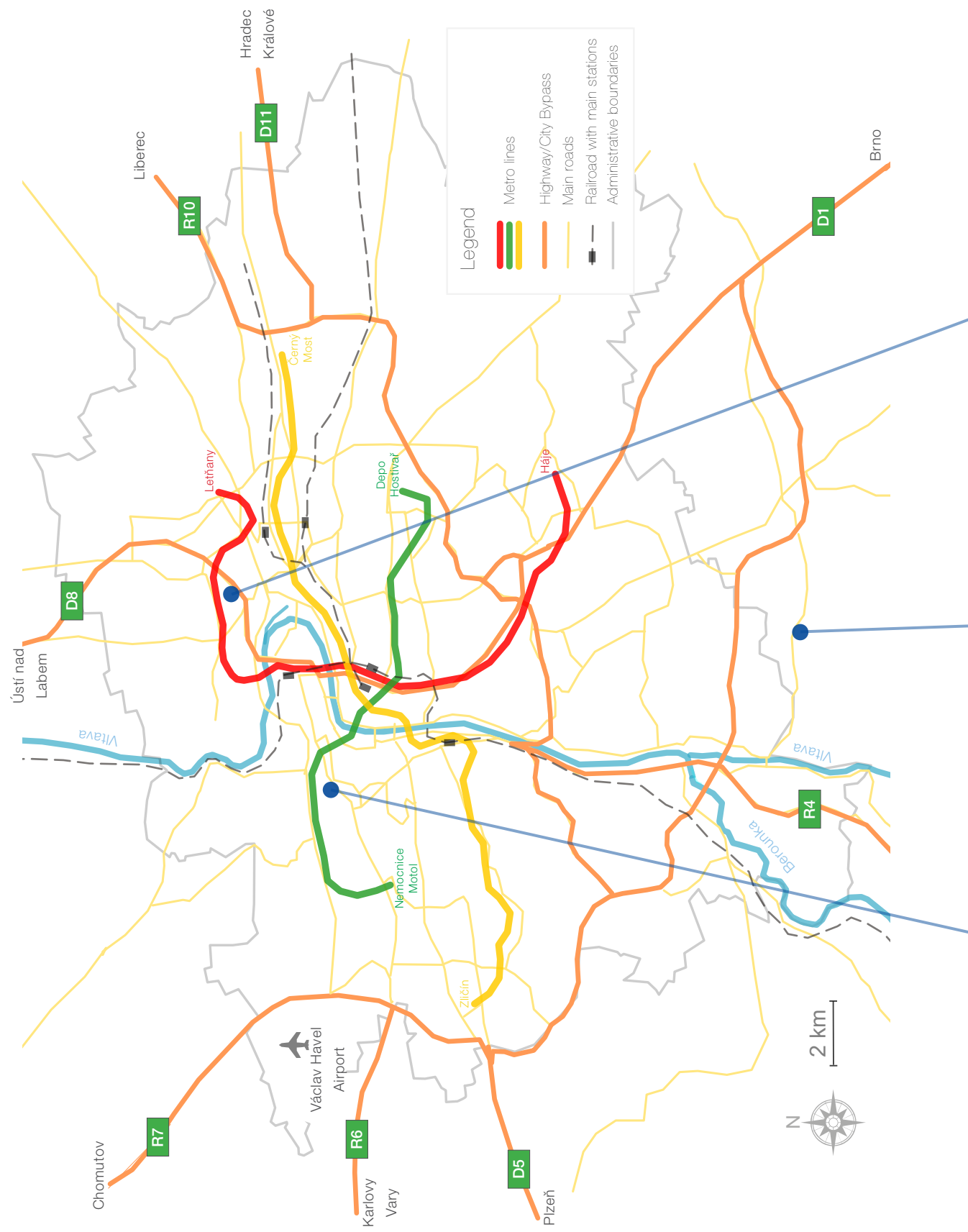
Activity Report

2010–2014

# Organizational Schema of the Institute of Physics



Research Division  
 Research Department  
 Research department, which is a part of joint laboratory (partner institution mentioned)  
 Support Department  
 Administration Department  
 \* Operational Program Research & Development & Innovations



Dolní Břežany



# Contact Info

## Main building Na Slovance

Division of Elementary Particle Physics, Division of Condensed Matter Physics, Division of Optics, Division of High Power Systems (Department of Radiation and Chemical Physics), Director, Central Section

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*For site location within Prague see the map on previous page.*

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Czech Republic

Phone: +420 220 318 510  
Fax: +420 233 343 184



## ELI Beamlines

ELI Beamlines Division

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252 41 Dolní Břežany  
Czech Republic

E-mail: [info@eli-beams.eu](mailto:info@eli-beams.eu)  
Website: [www.eli-beams.eu](http://www.eli-beams.eu)

## HiLASE

Division of High Power Systems  
(Department of Diode-Pumped Lasers)

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Czech Republic

Email: [radka.kozakova@hilase.cz](mailto:radka.kozakova@hilase.cz)  
Website: [www.hilase.cz](http://www.hilase.cz)







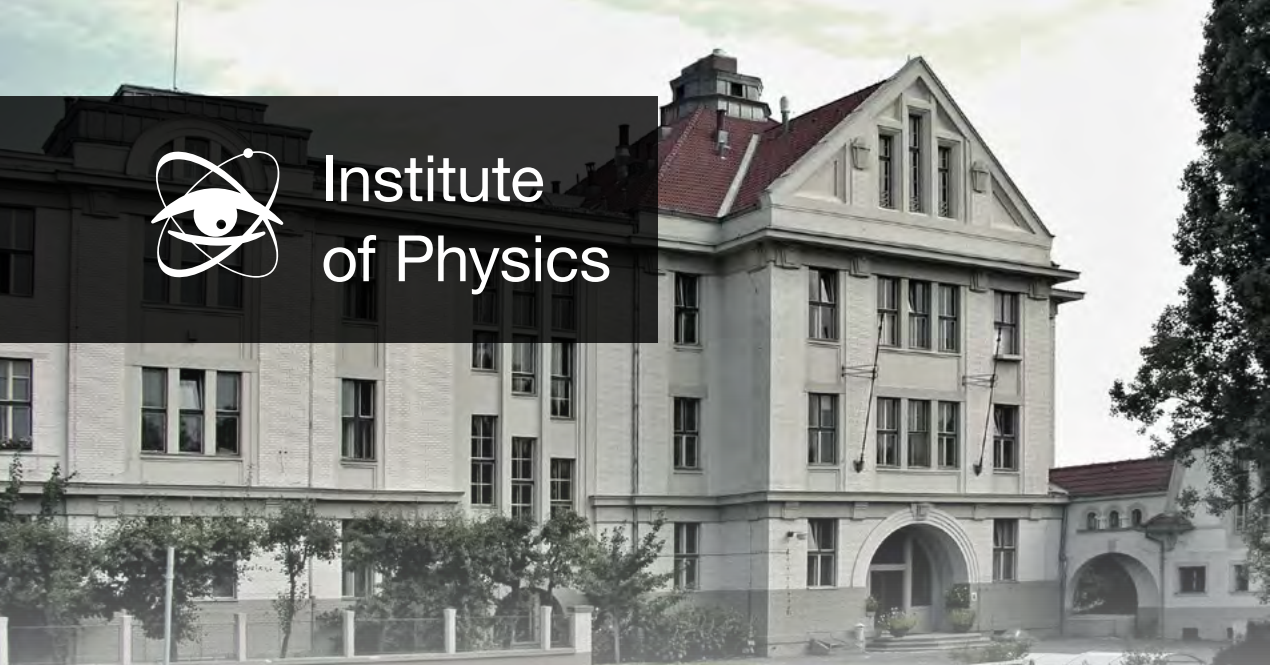
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Institute  
of Physics



# Introduction



The Czech Academy  
of Sciences





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## Foreword



Dear Reader,

The Institute of Physics (Fyzikální ústav AV ČR, v. v. i.) celebrated the 60th anniversary of its existence last year. This amount of time is quite significant given all the upheavals of the 20th century. Over a background of sometimes dramatic societal change, physics has kept evolving and our Institute has always tried to keep pace with its progress, and to contribute to its evolution. One of the most important developments after 1989 is the rapid growth of cooperation with many research institutions and universities from abroad.

An important legal change came in 2007 when the Institute became a public research organization. As a consequence, the Institute is obliged to publish annual reports, in a specified structure, in Czech. The aim of this Report is to summarize our activities over a longer period and bring them to the attention of a wider public. It is planned to issue similar summarizing reports regularly in the future. Our goal is to convey the complete picture of research at our Institute to all interested persons, and especially to our collaborators and colleagues from abroad, as individual cases of cooperation usually entail specialized teams and concern particular fields of physics. Given the size of the Institute — 1200 employees, 6 scientific divisions with 25 scientific departments, we would like to present the picture of the whole institute with the hope this will facilitate even wider successful cooperation in new and exciting topics.

Prof. Jan Řídký  
Director





A scientist wearing a white cleanroom suit and glasses is focused on adjusting a complex piece of scientific equipment. The equipment features various components, including a prominent green vertical section and a purple circular element. The background is a clean, bright laboratory environment.

Institute of Physics  
The Czech Academy  
of Sciences

Trends 2010–2014

## Introduction:

### The Structure and the Role of the Institute

Fyzikální ústav AV ČR, v. v. i. (FZÚ; in English: Institute of Physics of the Czech Academy of Sciences) is a public research institute, conducting fundamental and applied research in physics. The founder of the Institute is the Czech Academy of Sciences. The present research program of the Institute comprises five branches of physics: particle physics, physics of condensed matter, solid state physics, optics and plasma physics. The institute is divided into major research divisions corresponding to these branches.

Since January 1, 2007 the FZÚ has been a public research institution (v. v. i.). The Structural funds of the European Union significantly influence the research in the FZÚ, which is a coordinator of the greatest such project in the CR aimed at the Extreme Light Infrastructure (ELI). For its realization a new Division was created in 2012. The FZÚ is the largest institute of the Academy of Sciences of the CR, with more than 400 scientists.

FZÚ has always been an important center of international cooperation. Today, several of its laboratories are nodes in programs of European Community, and many more participate in international grant programs, bilateral co-operations, and the work of international research centers all over the world. A number of prestigious international conferences and schools organized by the Institute brought thousands of international experts to the Czech Republic. Within the country, the cooperation with other institutes of the Academy and with Czech universities has high priority.

Traditionally, graduate studies in physics have been a joint effort of the universities and of the Academy. Presently, the Institute of Physics is accredited to educate students in a number of fields, with the PhD degrees being granted by Charles University, Palacký University, Czech Technical University as well as other Czech technical and technological universities. Many of the graduate students nowadays come from abroad. Different support programs, including the Marie Curie Training Site, are available. In some areas, the needs of research cooperation prompted more profound steps towards uniting resources and coordinating the efforts. Within the Academy, and together with the universities, the Institute has helped to establish several Joint Laboratories, as well as several national Research Centers.

As we have stated above, FZÚ currently comprises six scientific divisions. The detailed organizational schema of the Institute is available on the inside of the front cover of this brochure. A brief overview of the current organizational division is described below:

#### Division of Elementary Particle Physics

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The accelerator experimental program of the Division is conducted within the **Department of Experimental Particle Physics** as well as the **Department of Detector Development and Data Processing**. The program of the **Department of Particle Theory and Phenomenology** focuses on a range of topics from purely theoretical and formal subjects within string theory to the phenomenological aspects of real-world hadrons – strongly interacting particles. **The Department of Astroparticle Physics** participates in the Pierre Auger Observatory and Cherenkov Telescope Array to study particles and photons with energies several orders of magnitude higher than those of terrestrial accelerators.

#### Condensed Matter Physics Division

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The **Department of Dielectrics** has traditionally been connected to the physics of ferroelectrics and structural phase transitions. The **Department of Advanced Structural Materials** currently focuses on development of new prospective bulk materials with controlled microstructure, including ultra-fine-grained metals with unique properties. The **Department of Functional Materials** focuses on studies of unique properties of materials exhibiting martensitic phase transformations, particularly NiTi shape memory alloys and ferromagnetic Heusler alloys. Furthermore, the departmental researchers also grow and characterize CVD nanodiamond films and particles for a broad range of applications in engineering, energy and medical fields. The **Department of Magnetic Nanosystems** is focused on studies of transition metals (magnetic nanoparticles, thin films, giant anisotropy materials) and carbon nanostructures in broad ranges of temperatures and magnetic fields. Research activity in the **Department of Condensed Matter Theory** is mainly focused on ab-initio calculations and modeling the electron properties of metals, semiconductors, and other complex materials with non-trivial elementary cell or with enhanced electron correlation effects. The **Department of Chemistry** focuses on material technologies such as crystal growth, sample preparation, chemical analysis and synthesis of liquid crystals.

## Division of Solid State Physics

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The **Department of Structure Analysis** builds on a long history of the X-ray physics research where the understanding of atomic structure, electron states and hardness enables research into unique materials. The principal technology used in the **Department of Semiconductors** is the Metal-Organic Vapor Phase Epitaxy (MOVPE) which makes it possible to prepare unique nanostructures, such as quantum dots and wells. Molecular Beam Epitaxy (MBE) and Electron Beam Lithography (EBL) are two basic technologies of the **Department of Spintronics and Nanoelectronics** which enable, together with theoretical background, a study of a series of phenomena pertaining to a fast developing branch of research, spintronics. The **Department of Thin Films and Nanostructures** focuses on the study of amorphous silicon, used in flat screens or photovoltaic cells. Within this department, research into the surfaces and silicon nanocrystals naturally led to the development of nanotechnologies and/or nanophotonics, while Atomic Force Microscopy and Scanning Tunneling Microscopy (AFM/STM) and unique methods of theoretical calculations enabled visualization, identification as well as targeted formation of nanostructures on an atomic level. Preparation and study of various forms of diamond are an important part of the research of the **Department of Optical Materials**. Considerable attention is also paid within this department to scintillation materials, studied in the frame of many national and international co-operations.

## Division of Optics

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The **Department of Optical and Biophysical Systems** is mainly focused on the research and development of optical materials and systems for micro-electronic, optoelectronic and biomedical applications. Quantum optics with cryptographic applications and nonlinear optical phenomena are investigated at the **Joint Laboratory of Optics** which is considered as a Department in the organizational scheme of the Institute. This department has, for a long time, dealt with advanced approaches and applications focused on various areas of applied and technical optics and optoelectronics, most notably for large astroparticle physics experiments as in the Pierre Auger Observatory or the Cherenkov Telescope Array. Advanced characterization of materials is performed at the **Department of Analysis of Functional Materials**, which is a part of the Center for Analysis of Functional Materials (SAFMAT). The research of low-temperature plasma deposition processes at the **Department of Low-Temperature Plasma** is oriented to the development of the plasma reactors, used for the deposition of advanced thin film structures.

## Division of High Power Systems

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The **Department of Radiation and Chemical Physics** studies phenomena on the edge of high energy density physics and also high energy chemistry, particularly the interaction of extremely intense ultraviolet and X-ray radiation with matter. The key project of strategic importance is the construction of a modern laser research centre HiLASE in Dolní Břežany driven by the **Department of Diode Pumped Lasers**. This project is focused on the experimental development of a new generation of diode-pumped solid-state lasers with high pulse energy and high repetition rate.

## ELI Beamlines Project Division

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This division has a very specific role. It has as its main goal, preparation and realization of the ELI (Extreme Light Infrastructure) Beamlines project, which is the largest research initiative in the history of the Czech Republic. The research projects at ELI will cover the area of interaction of matter with light at extreme intensities, about 10 times higher than current limits. ELI will provide ultrashort laser pulses of a few femtoseconds (10-15 fs) duration and give performance of up to 10 PW. Although ELI Beamlines is already divided into several departments, we present it here in this brochure as one unit. This division was only established in 2012, and the project is still in its construction phase, therefore the research output of this division is still naturally quite small.

The vertical organization of FZÚ extends from divisions, as they are described above. The smaller divisions are of the size of about 80 FTEs, which corresponds to smaller Academy institutes. Each division is then divided in several departments, and departments may be divided into several teams/groups. The teams in the structure of FZÚ may be quite small and will have the basic attribute of one single common research goal and a team leader who is responsible for the work of the team. Usually such a team is supported by one grant project and the team could possibly span across different departments or divisions. These teams are easy to establish or dissolve from an administrative point of view. The team leader has as few administrative duties as possible and his/her lead could be quite informal. In contrast with that, the department lead has a number of administrative duties (budget of the department, reports, hiring and personnel issues etc.) and he/she is responsible also for the supervision of the teams in his/her department. Division leaders then participate on the governance of the Institute.



## Human Resources

The age structure of all employees, and of research employees, respectively is shown in the two accompanying graphs. The gap in the age period 45-60 years, present in the both plots is a remnant from the first half of 90s, when after the fall of the communist regime the Institute was reduced from 1 200 employees to 600 and many employees of productive age left the Institute to pursue careers in the newly opened private sector. In this critical period also, many university students were attracted to study economy and law which provided superior career opportunities at that time. The influx of new PhD students to the Institute was thus much lower than needed. The resulting gap now propagates gradually towards retirement age.

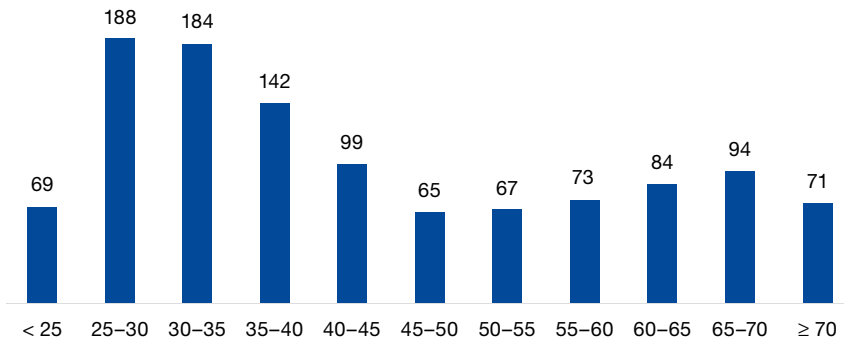


Fig. 1: Age structure of all Institute employees

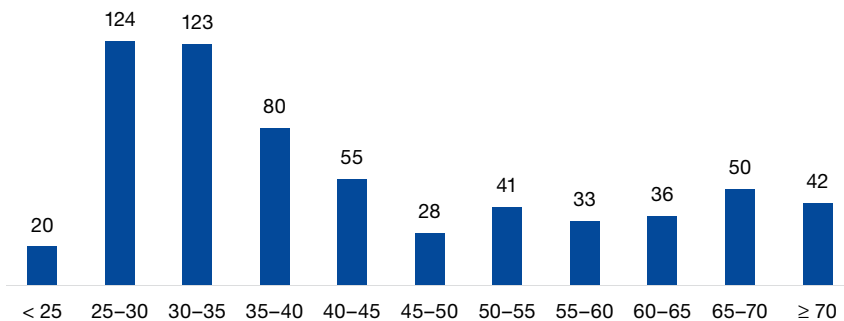


Fig. 2: Age structure of research employees (researchers, doctoral students, other research employees)

Realization of the two big projects ELI and HiLASE started in 2010. This is reflected in the graph below. The two projects caused an increase of the staff by about 300 employees. The rest of the increase is related to the remaining part of the Institute. The graph also depicts the qualification structure where the category “researchers” includes both researchers and senior researchers, the category “PhD students & others” encompasses PhD students, postdocs and assistant researchers.

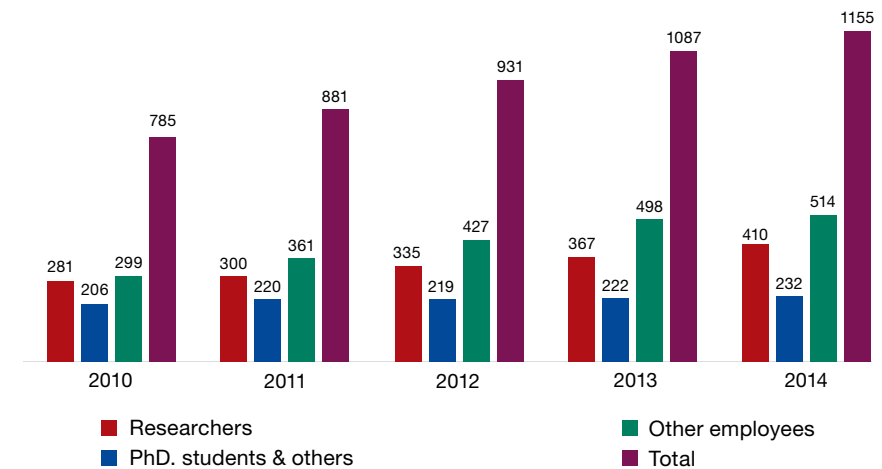


Fig. 3: Gradual growth of the number of employees

The two big projects ELI and HiLASE also changed the Institute structure in terms of international representation (see fig. 4 illustrating this aspect). Of course the influx of foreign staff members is almost entirely in research categories.

The evaluation of researchers is based on a yearly attestation process. By Academy rules each employee in a research position has to pass this process at least once every five years. Evaluation criteria consist of publication activity, citations index, grant activity, lecturing at universities and PhD supervision, contractual research, patents, outreach etc. The statement of the employee’s superior is also provided. The materials are reviewed by the attestation committee consisting of six division leaders and four external members, two of these from universities and two from other Academy institutes. The employees considered to be on a critical path are usually called to attestation in a one or two year period.

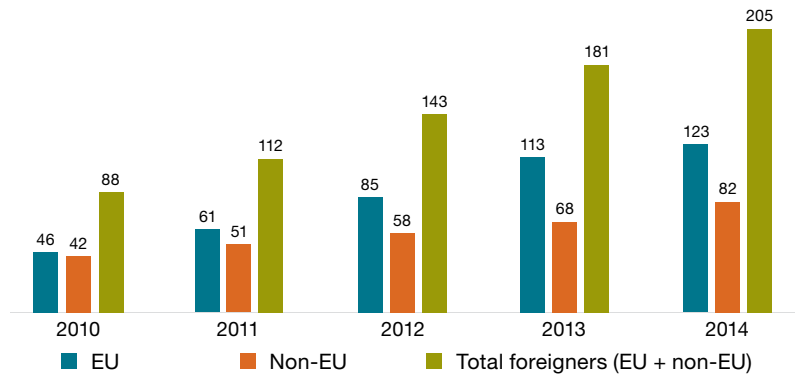


Fig. 4: The increasing number of foreign research employees

Hiring of new employees was done in almost all cases by invitation for applications. Career development follows the recommendations of the attestation committee. Regarding career development one should note two important tools provided by the Czech Academy of Sciences (CAS) are used. Namely Praemium Academiae (PA) and J. E. Purkyně Fellowship (FJEP). Besides these there are other two CAS instruments for financial support of PhD students (Premium of Otto Wichterle) and postdoc support. In general, the Institute strongly encourages fresh postdoctoral researchers to spend at least one year or more abroad at a research institution or university. This should be a crucial condition to continue a career in the Institute.

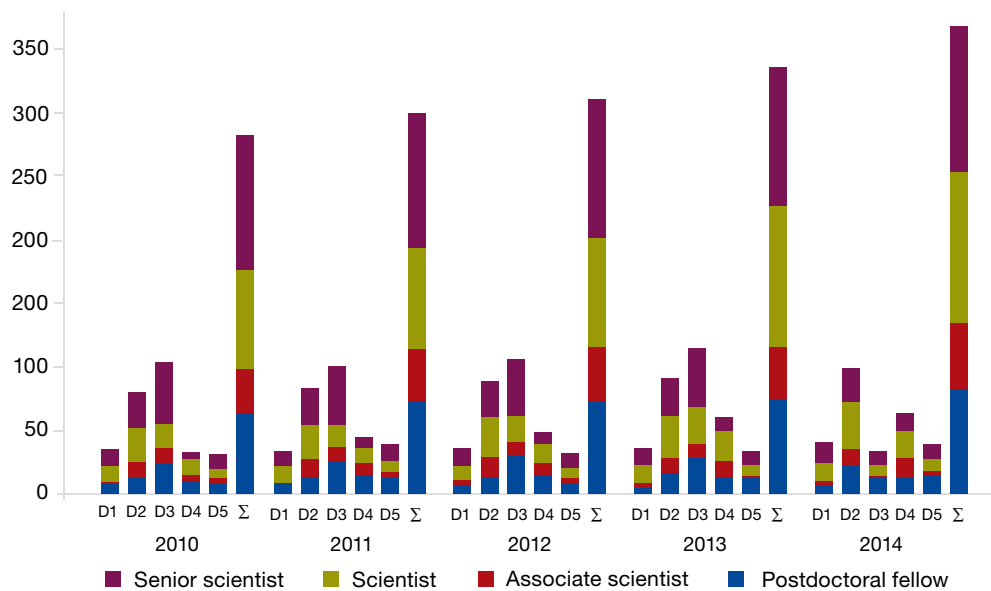


Fig. 5: Number of scientists as divided into individual divisions and individual research grades (not including PhD students and research assistants) – except the ELI Beamlines Division.

## Budget

The budget of the Institute consists of two basic components – the institutional part that is being provided by the state through the Academy of Sciences, and the targeted part that is provided through various national and international grants and projects. The institutional part of the budget is currently about one half of the total budget, but it should cover the largest part the base salaries and running costs of the Institute. The targeted research represents the other half of the budget. Most finances for this come from various grant agencies for particular specified projects, mostly from Czech Science Foundation (CSF) and to a lesser extent from the Technology Agency of the Czech Republic (TACR) and a minor but important section are derived from the EU schemes (FP6, FP7, ERC).

The “disposable income” of the institute is thus very limited. The graph inserted below shows the institutional part of the budget. After a dramatic decrease between 2009 and 2010 the overall institutional budget oscillates around 300 mil. CZK and it has never regained previous value. This trend is rather contradicting the rapid development of the Institute thanks to the activities financed from the Structural funds of the EU during the last few years.

Even in these circumstances there is clear correspondence of our research themes with recent trends in various domains of physics, e.g. a more pronounced focus towards bio-oriented problematics. However, with a higher institutional budget (even at the expense of targeted research) catching up with the research trends could be more rapid. Targeted research is quite expensive in terms of human resources.

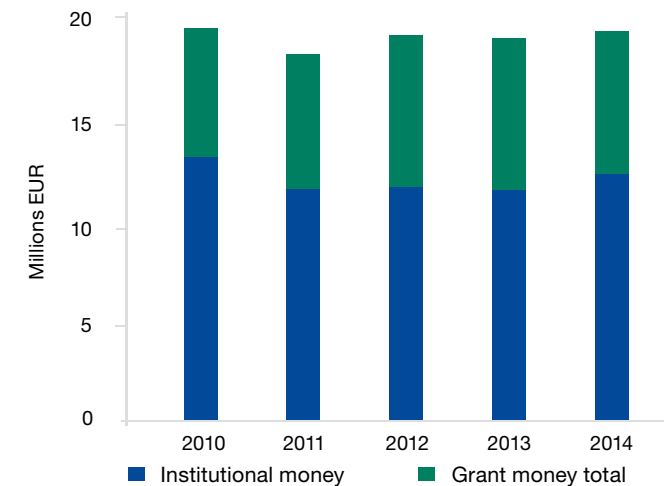
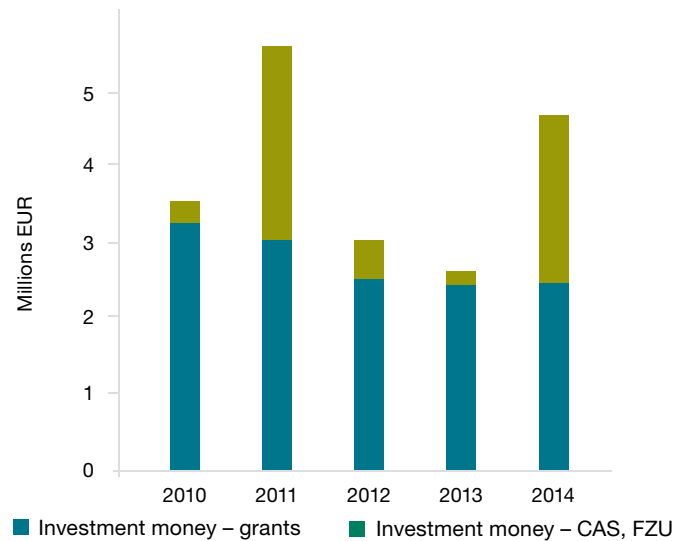
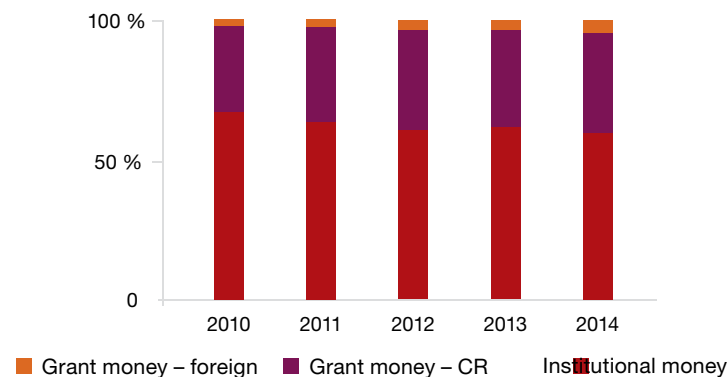


Fig. 1: Operational budget – except the ELI Beamlines Division. Exchange ratio used for the plot: 1 EUR = 27.5 CZK

Despite a not quite optimal structure of the budget the Institute can cover urgent financial needs up to a certain limited amount. Naturally this limit corresponds to the size of the budget, hence also to that of the Institute – as a large institute the FZÚ thus has much better ability to solve such urgent financial needs.



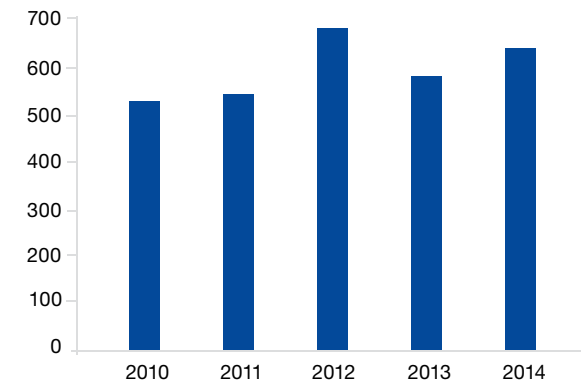
**Fig. 2:** Investment budget – except the ELI Beamlines Division  
Exchange ratio used for the plot: 1 EUR = 27.5 CZK.



**Fig. 3:** Operation budget – except the ELI Beamlines Division

## Publications and Other Scientific Outputs

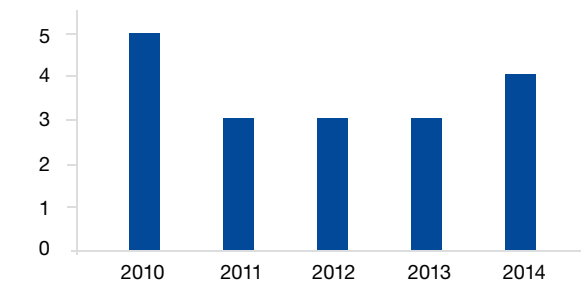
As the most of the activities of the Institute are dedicated to fundamental research, the most typical scientific outputs are papers in the international peer-reviewed journals. One of the criteria that characterizes the effectiveness of the scientific work is the number of such papers in high impact journals. The plot illustrating the development of the number of publications during the last five years is shown on right. The total number of papers is influenced by the activities of large international collaborations in particle



**Fig. 1:** Number of published papers in impacted journals

physics. Specifically, the number of papers published by scientists from the Division of Elementary Particle Physics has been, in recent years, closely linked to the activity of LHC in CERN. With the LHC running, the number of papers in this division is over 200, but during the LHC technological break, the number of papers of this division decreased to about 100. When we take into the account that a significant part of the institute is currently undergoing the construction phase of its crucial facilities (ELI Beamlines, HiLASE) and thus the publication activity is somewhat limited, we arrive at a very healthy estimate of 2 publications per scientist per year.

The co-operation with the industry and the focus of certain activities at FZÚ to applied research, results in outputs that are not publications, but rather patents or utility designs. The number of awarded national patents in individual years is plotted below. It should be noted that the patent acceptance procedure usually takes several years, and thus recent improvements in this area (e.g. the activity of the CITT center) is not yet influencing the given plot.



**Fig. 2:** Awarded Czech national patents



## Pedagogical Activities

Fyzikální ústav AV ČR, v. v. i. has an intensive collaboration with more than 10 Czech universities as well as with many universities abroad. Not surprisingly, the strongest collaboration of the Institute is with Charles University in Prague, with Palacký University in Olomouc and with the Czech Technical University in Prague, which are all our research partners with a very long tradition of co-operation. Most PhD students come to FZÚ from these three universities.

Type of study	No. of supervisors (theses, dissertations)	No. of consultants or co-supervisors	Theses defended in 2010-2014
Bachelor	67	25	86
Master	81	38	90
Doctoral	118	98	85

The research employees of the Institute are also very active in direct teaching duties at about seven different universities in the Czech Republic. These are again most prominently active at Charles University in Prague, the Czech Technical University in Prague and Palacký University in Olomouc. Teaching activities of employees are also strongly supported by the FZÚ management. Several tens of research employees are actively involved in teaching.

As an illustration of the level of the teaching activity, we evaluate below the number of lecturing hours in various programs during the both semesters of the last academic year: During the summer semester of the year 2013/2014 researchers conducted 1076

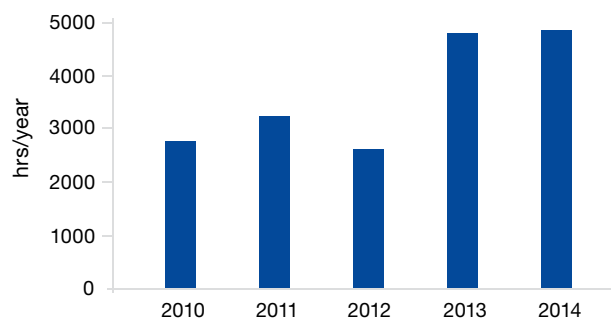


Fig. 1: Lecturing at universities

hours of lectures in bachelor programs, 890 hours in master programs and 217 hours in PhD programs. In the winter semester 2014/2015 the totals were 1047 hours in bachelor programs, 1252 hours in master programs and 383 hours in PhD programs. The FZÚ employees participated in lectures in almost 200 separate university courses.

One of the primary goals of the management of the FZÚ is to turn the Institute into an excellent training center for PhD students in collaboration with Czech universities. The ultimate goal is that, in the foreseeable future, the interest of students in enrolling into PhD training in FZÚ due to the excellent quality of the PhD training will surpass the number of available positions, and that the government and industrial companies will eventually support PhD training at FZÚ. After this is achieved, an internal grant system for PhD training will be introduced in the FZÚ to select the best PhD candidates.

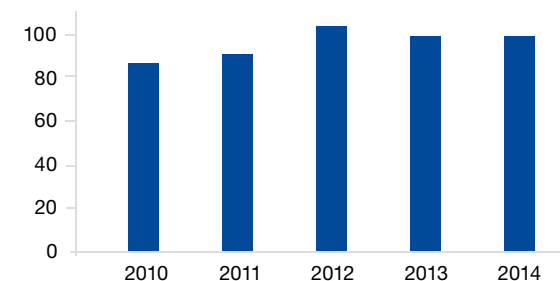


Fig. 2: Number of PhD students

To achieve this goal, PhD education at FZÚ has been centrally organized since 2012, the quality of individual PhD programs has been evaluated on a yearly basis using a “PhD evaluation procedure” held annually in November. The course of each PhD study is reviewed and the results are evidenced in the online database EVDOK. The quality of the PhD training, not the student is evaluated. The approved PhD programs are supported financially either from the institutional or from the project budgets.

## Research Popularization and Editorial Activities

In 2010–2014, the scientists of the Institute have been also very active in the area of research popularization.

From a long-term perspective FZÚ collaborates with many high school students (and in some cases even with elementary school pupils) on both a formal and informal basis. There is very popular program organized by the Czech Academy of Sciences called Otevřená věda (Open Science) that enables a selected high-school student to start a collaboration on a research project directly with the Institute. The results of the projects are then presented and evaluated during the annual science fair. Several tens of these Open Science projects were led by FZÚ employees during the evaluation period. FZÚ researchers serve also as reviewers, judges and consultants in various other high-school competitions such as the Středoškolská odborná činnost

(High-school research projects), the International Physical Olympiad or the International Young Physicist Tournament. Many of the researchers also lecture directly at the high-schools and elementary schools.

The collaboration with the popular science magazine with largest circulation, *Vesmír* (*The Universe*), is also very intensive. Several employees are members of the editorial board of the national astronomical magazine *Astropis*. Many scientists contribute also to two magazine issued directly by the Institute, for these activities see the next section of this report. There is also broad collaboration the public radio station – *Český rozhlas*, most notably with the very popular and science-dedicated broadcast, *Meteor*. Many scientists have also participated in another broadcast, *Studio Leonardo*.

The FZÚ researchers have also made frequent appearances on national TV, most notably in discussion programs such as *Hyde Park*, or on the news channel TV24. The Institute frequently contributes to the news site of the Academy, and also has its own very active web portal, maintained both in Czech and English.

Several of the most important personalities in the Czech Republic in the area of science popularization are active at the Institute. Most notably, Jiří Grygar, who is possibly the best recognized scientist in the Czech Republic. He is known by general public mostly for his highly influential popular book and TV series *Okna vesmíru dokořán* (*Windows to Universe Wide-Open*). Other researchers from the area of particle physics are widely cited in many popular publications, e.g. Jiří Chýla (known also for his blog devoted mostly to science financing), Jiří Rameš, Martin Schnabl, Petr Trávníček and Michael Prouza. Many of scientists in other branches of physics also devote a large part of their time for the popularization of science, e.g. Antonín Fejfar, Pavel Jelínek, Tomáš Jungwirth, Martin Nikl, Libor Juha (also the editor-in-chief of the Institute's journal *Československý časopis pro fyziku*) and Tomáš Mocek.

The Institute publishes two semi-popular journals that publish papers which sit at an intermediate level between popular science and true research publications. Both journals have a very long tradition and several hundred subscribers in the Czech Republic, especially in the community of high-school physics teachers. Many professionals also subscribe these journals and access is free for all employees of the Institute. General physics news, special reports and interesting articles from the history of physics are covered by the *Československý časopis pro fyziku* (*The Czechoslovak Journal for Physics*, as distinct from the previous English research journal). *Čs.čas.fyz.*, as it is commonly known, exists in this form since 1951, and under the leadership of the current editor-in-chief Libor Juha, it was largely modernized and has now a professional layout and DTP.

The second journal *Jemná mechanika a optika* (*Precision Mechanics and Optics*, abbreviated to *JMO*) is dedicated mostly to the issues of optics and precision mechanics. Some of the articles published here might be considered as a research papers, others are summaries of interesting topics, news from conferences, etc. The journal is issued in close collaboration with the private company Meopta producing optical instruments. Books are not issued by the institute directly, but the authors collaborate closely with the most prominent and prestigious publishing houses – *The Econophysics* by František Slanina published by Oxford University Press in 2014 and *Grain Boundary Segregation in Metals* by Pavel Lejček published by Springer in 2010 might serve as examples.

Many researchers also serve on the editorial boards of important international physics journals, or serve as the editors of the special issues of journals.

## Dvořák Lectures

To commemorate work and personality of prof Dvořák, former director of the Institute (more on p. 240), the Institute organizes an annual festive Dvořák lecture, given by prominent internationally renowned scientists in the field related to the research pursued at the Institute of Physics.

### Dvořák Lectures in last years

- 2009** ■ Yoshihiro Ishibashi (Nagoya University, Japan)  
Thermodynamic Approach to Nano-Inhomogeneous Ferroelectrics
- 2010** ■ Anton Zeilinger (University of Vienna, Austria)  
Quantum Information and the Foundations of Quantum Mechanics
- 2011** ■ Dieter Vollhardt (University of Augsburg, Germany)  
Superfluid Helium-3: From very low Temperatures to the Big Bang
- 2012** ■ Allan H. MacDonald (University of Texas at Austin, USA)  
Graphene Ten Years later
- 2013** ■ Peter Jenni (University of Freiburg, Germany; CERN, Geneva, Switzerland)  
The long journey to the Higgs boson and beyond at the LHC
- 2014** ■ Orazio Svelto (Politecnico di Milano, Italy)  
The LASER: a Historical Perspective



Institute of Physics  
The Czech Academy  
of Sciences

History  
of the Institute



The **Institute of Physics of the Czechoslovak Academy of Sciences (CSAS)** was formally established by merging of the **Laboratory for Nuclear Physics (LNP)** CSAS and the **Laboratory for Experimental and Theoretical Physics (LETP)** CSAS in 1954. Therefore, our institute celebrated the 60th anniversary of its existence last year, in 2014.

However, the present-day structure of the Institute is a result of many important events both before and after this crucial milestone. Firstly, both the LNP and the LETP had been already established two years earlier as parts of the newly created Czechoslovak Academy of Sciences. While the LETP was created anew in 1952, the LNP was a successor to the **Institute of Atomic Physics** of the Czech Academy of Sciences and Arts founded in 1946. Shortly after the merger, in 1955, a part of the Institute of Physics, residing in Hostivař, split off and formed the basis of the future **Institute of Nuclear Physics (INP)** CSAS.



**Fig. 1:** The complex of the Research Institute of the Czechoslovak Sugar Industry (RISI) in Cukrovarnická street (Střešovice) was built during 1920–1923 and acquired by the Central Physical Institute in 1951



**Fig. 2:** The building in the street Na Slovance was built for the needs of the growing Institute of Physics which moved there in 1970

Another lineage of physical research dates even further back, to 1932, when the **Institute for Physical Research of the Skoda Factory (IPRSF)** was founded to satisfy the research needs of the Skoda factory in Pilsen in cooperation with the Spectroscopy Institute of the Charles University. This organization then went through a series of changes in both structure and name. First, it was nationalized and renamed the **Central Physical Institute (CPI)** in 1950 – a title that lasted only two years as the birth of the CSAS in 1952 meant that the CPI was included in its newly formed structure as the **Institute of Technical Physics (ITP)**; only to be renamed the **Institute of Solid State Physics (ISSP)** ten years later.

Finally, these two stories converged in 1979, when the Institute of Physics merged with the ISSP and also the **Low Temperature Department** of the Institute of Nuclear Physics (INP) CSAS – the very same institute that emerged by splitting off the Institute of Physics in 1955. This major merger marks the beginning of the Institute of Physics in its present form; since then it is important to note the incorporation of the **Department of the Applied Plasma Physics** of the Institute of Plasma Physics (IPP) CSAS in 1983 and the gradual creation of several joint laboratories with other Czech research institutions.



The Velvet Revolution in 1989 brought important changes not only in the freedom of the scientific research, but also in management of the Institute. In 1990 the Division of Optics was created, an important part of which has been, since 1985, the Joint Laboratory of Optics of the Institute of Physics and Palacký University in Olomouc, one of the first joint laboratories between the Institute and the University.

Since January 1, 2007 the Institute of Physics has become a “public research institution” (v. v. i.). In recent years, the Structural funds of the European Union significantly have influenced the research in the Institute, which is a coordinator of the greatest such project in the Czech Republic aimed at the construction of Extreme Light Infrastructure (ELI) in Dolní Břežany near Prague. A new Division was created in 2012 for the realization of the ELI Beamlines project.



**Fig. 3, 4:** New buildings of ELI project in Dolni Brezany

Next to the building of ELI in Dolní Břežany is located the second modern laser center of the Institute of Physics – HiLASE. This project was driven by the Division of High Power Systems and started operation in 2014. It was also financed using the resources of the EU Structural funds. Other newly opened laboratories also took advantage of the EU Structural funds – e.g. the Center of Analysis of Functional Materials (SAFMAT), Center of functional materials for bio-applications (FUNBIO), and the Laboratories for preparation and characterization of nitride semiconductor heterostructure (LABONIT) and Advanced Structure Analysis (ASTRA).

The Institute of Physics is currently the largest institute of the Czech Academy of Sciences, with more than 400 scientists.



**Fig. 5:** New building of HiLASE



Institute of Physics  
The Czech Academy  
of Sciences

Laboratories and  
Technology Transfer



## Experimental Facilities and Central Laboratories

The institute hosts world-class experimental and computational facilities for characterization of structural, chemical and physical properties of materials, dedicated facilities for processing and testing of materials as well as range of technologies for preparation and processing of materials. This equipment is installed within multiple scientific departments. The dedicated website <http://xroads.fzu.cz> has been launched to provide structured links, access information and details on the equipment.

FZÚ runs eight central laboratories offering research services in the area of materials research (surface analysis, electron microscopy, high power laser technology, x-ray diffraction, structure analysis, physical property evaluation, chemistry and laser physics experiments) to its scientific teams as well as to the wider research community.

- SAFMAT — Centre for Analysis of Functional Materials [safmat.fzu.cz](http://safmat.fzu.cz)
- LNSM — Laboratory of Nanostructures and Nanomaterials [lnsm.fzu.cz](http://lnsm.fzu.cz)
- HiLASE — New Lasers for Industry and Research [www.hilase.cz](http://www.hilase.cz)
- ROTAN — Laboratory ROTAN [rotan.fzu.cz](http://rotan.fzu.cz)
- ASTRA — Advanced Structure Analysis [astra.fzu.cz](http://astra.fzu.cz)
- JLMS — Joint Laboratory for Magnetic Studies [kfl.cz/jlms](http://kfl.cz/jlms)
- Laboratory of Chemistry [xroads.fzu.cz/laboratories/laboratory-chemistry](http://xroads.fzu.cz/laboratories/laboratory-chemistry)
- PALS — Prague Asterix Laser System [pals.cas.cz](http://pals.cas.cz)

## Research Commercialization

The institute runs a Technology Transfer Office CITT (<http://www.citt.cz>) with the aim of supporting commercialization of its research results. The number of patents and research collaborations of FZÚ teams with industry have been steadily growing in recent years. CITT supports FZÚ scientists in the effort to find engineering applications for their results. In particular it tries to establish new contacts with the industry for its research teams, ensures protection of intellectual property rights, evaluates legal and financial aspects of the collaboration with industrial partners, and provides means for advertising, marketing and promoting the research results.

A new research commercialization program has been launched within the institute in 2015–19 in frame of the national technology transfer project GAMA TACR. Within this unique project, FZÚ research teams which already achieved applicable results are provided with financial and administrative support to commercialize those results.

FZÚ central laboratories (<http://xroads.fzu.cz/laboratories>) offer open access research services to the industry and academia particularly in the area of surface chemistry analysis, electron microscopy, structure analysis, x-ray diffraction and laser experimentation.

The recently founded HiLASE laser center (<http://www.hilase.cz/>) represents a major step by the institute towards applied research. This center focuses on the development of advanced high power, high repetition rate, diode pumped solid state laser systems for application in industry, such as lasers for micro-machining technologies, testing resistance of optical materials, cutting, welding, removal of deposits and laser shock peening.



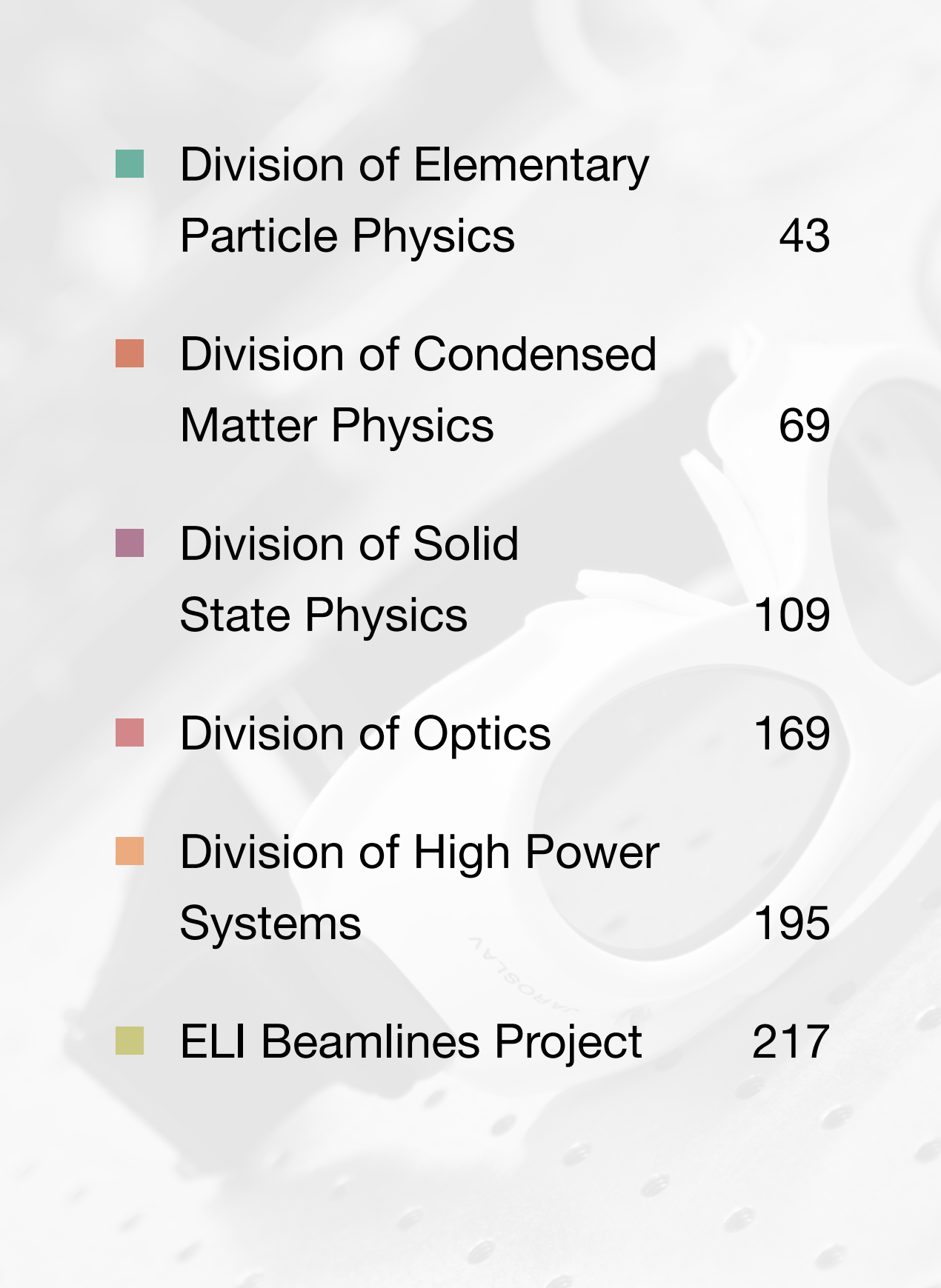
Institute  
of Physics

# Research

# Highlights

The Czech Academy  
of Sciences





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Institute of Physics  
The Czech Academy  
of Sciences

Division of Elementary  
Particle Physics



The research programme of the division is carried out mainly within large international collaborations which run their experiments in a few main research centres equipped with powerful accelerators. The principal purpose of these experiments is to study the structure of matter at the subnuclear scale and the properties of fundamental forces acting among its constituents.

The experimental programme of the division is focused on the ATLAS experiment at the LHC collider at CERN, France/Switzerland, the neutrino experiment NOvA at Fermilab, USA, and the experiments from the realm of astroparticle physics – the Pierre Auger Observatory in Argentina and the Cherenkov Telescope Array. This illustrates one of the most remarkable features of contemporary physics – ever-deeper connection of the laws of microcosm with the phenomena of macrocosm as traditionally studied by astrophysics.

Experimental activities of the divisions exploit the facilities and personnel of our Laboratory for semiconductor detectors. An integral part of our programme is also many-sided theoretical research ranging from string field theory and quantum gravity to the phenomenological aspects of strongly interacting particles.

The Division consists of four departments:

- Department of Astroparticle Physics p. 45
- Department of Detector Development and Data Processing p. 51
- Department of Experimental Particle Physics p. 56
- Department of Particle Theory and Phenomenology p. 61

## Department of Astroparticle Physics

The Department of Astroparticle Physics was created in 2010 as a consequence of the constantly increasing contribution of the institute to major international astroparticle physics projects. The institute has been successfully participating in prestigious astroparticle physics experiments for many years. Institute engineers and scientists helped to build, operate and analyze data of several international instruments such as CAT and CELESTE in the Pyrenees and the Pierre Auger Observatory installed in Argentina. In all these experiments our personnel took over at least partial responsibility for the design, construction, operation and maintenance of the segmented mirror telescopes. The involvement in prestigious astroparticle physics projects is based on close collaboration between the Division of Elementary Particles (Prague) and the Joint Laboratory of Optics of Palacky University and the Institute of Physics CAS (Olomouc).

Currently, the most important activities of the Department of Astroparticle Physics are the participation in the world's largest detection system of ultra-high energy cosmic rays – the Pierre Auger Observatory and the involvement in the preparation of a new observatory of high energy photons – the Cherenkov Telescope Array (CTA). Other activities in 2010–2014 concerned the laboratory measurements of fluorescence yield in air, which is crucial for precise energy reconstruction in fluorescence detectors, and participation in the pioneering project attempting to detect cosmic ray showers at gigahertz frequencies. Furthermore, the departmental staff take part in the project of the new largest survey telescope (LSST), which among other priorities aims to determine properties of dark energy and dark matter. Each year the projects of astroparticle physics as developed in our Institute and especially the Pierre Auger Observatory and the CTA Observatory attract new students from Charles University, Palacky University and the Czech Technical University.

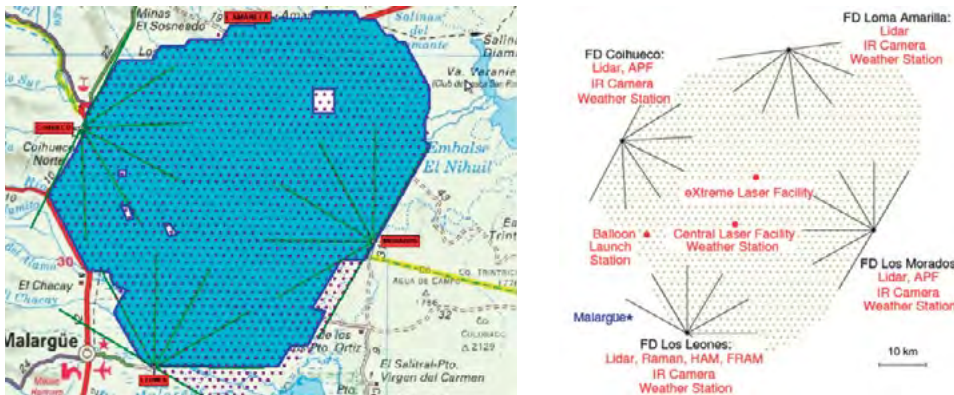
## Research Highlights

### Ultra-High Energy Cosmic Rays

The highest energy cosmic rays coming to the Earth from the Universe have been one of the most intriguing puzzles of modern physics for more than 40 years. These cosmic particles have an energy above 10 million trillion ( $10^{19}$ ) electron volts (eV). One would need to increase the beam power of the LHC, the world's largest particle accelerator, by a million times, to achieve energies as high as these remarkable cosmic rays. There is no scientific consensus on how or where cosmic rays with these ultra-high energies originate. Cosmic rays with energies above  $10^{19}$  eV arrive on Earth at a rate of only one particle per square kilometer per year. The especially interesting cosmic

rays, which have energies of over  $10^{20}$  eV have an estimated arrival rate of just one per square kilometer per century. In order to record a large number of these events, the Auger Observatory has created a detection area in western Argentina of the size of 3 000 km<sup>2</sup> – see Fig. 1.

With unprecedented collecting power and experimental controls, the Pierre Auger Observatory gathers the data needed to solve several important questions, namely: Where do these particles come from? What are they (composition)? How are they accelerated (source mechanism)? Does their energy spectrum end?



**Fig. 1:** The Pierre Auger Observatory, dots show the positions of surface detector stations. Also shown are the four fluorescence detector buildings on the perimeter of the surface array with 24 telescopes indicated. The battery of atmospheric monitoring instruments is listed superimposed in red in the right picture.

The Pierre Auger Observatory measures so called cosmic ray showers, which develop in the atmosphere as a result of an interaction of a primary cosmic ray particle coming from universe with the atomic nuclei of air gases. The institute joined the international collaboration in its early days in 1999 and participated in the design and prototyping as well as the construction of the observatory. The main hardware contribution of the group was the design and production of 15 out of 27 (12 m<sup>2</sup>) segmented mirrors of the fluorescence detector. Scientific topics connected with the fluorescence detector have remained the main part of the department's interest for many years. A member of the institute group served as the Fluorescence Detector Task Leader at the observatory. The unprecedented summarizing paper concerning the fluorescence detector of the Pierre Auger Observatory was written under the leadership of the institute group [1]. The alarm system developed by the department as well as the online cloudiness cameras from Olomouc helps to improve the data acquisition by the observatory. The department staff are involved in the operation of the fluorescence telescopes, the data analysis and the atmospheric monitoring [2].



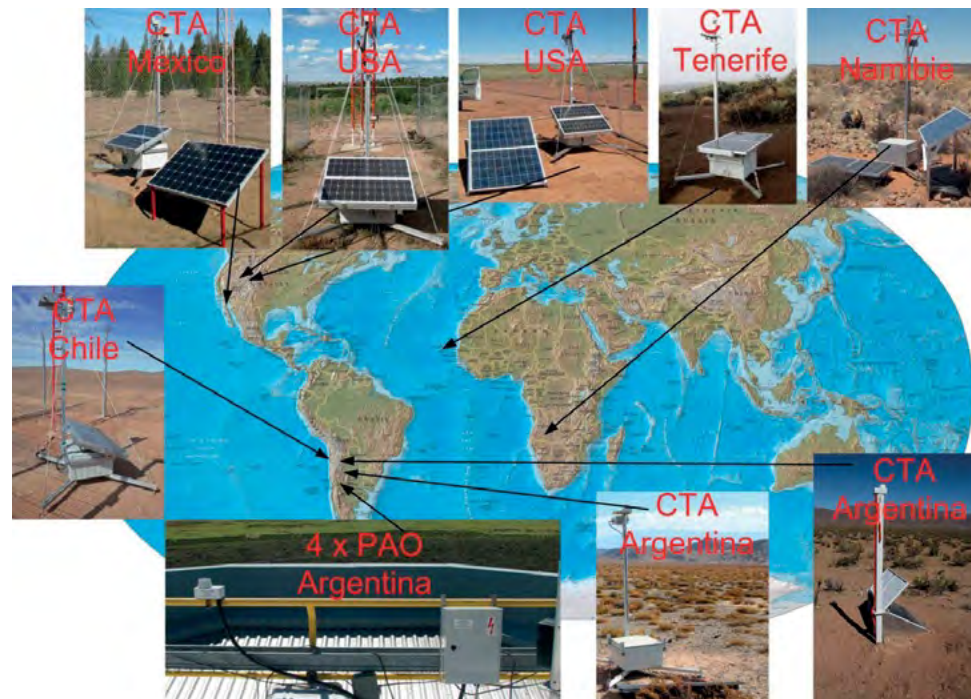
**Fig. 2:** FRAM (F/Photometric Robotic Atmospheric Monitor), seen here next to the Los Leones fluorescence telescope building is a robotic astronomical telescope capable of automatic monitoring of atmospheric conditions in various parts of the sky, including fast follow-up observations along the trajectory of a recently observed air shower. The telescope, its supporting infrastructure and the operating software have been developed by the Institute.

The monitoring of atmosphere (see Fig. 2) is essential for an unbiased shower reconstruction. Scientists in the department attempt to understand, how the properties of hadronic interactions [3] taking place during the shower development influence the shower properties, and which sources and processes are responsible for an origin of high-energy cosmic particles [4], how these particles propagate through the universe to the Earth [5] and the composition of cosmic rays [6, 7]. The involvement in the Pierre Auger Observatory is one of the key projects of the institute and an example of the successful world-wide collaboration of our scientists with foreign institutions. This participation has in fact driven to a large extent, the establishment of a new research field (of astroparticle physics) for the Czech Republic. The department also takes part in the planned observatory upgrade.

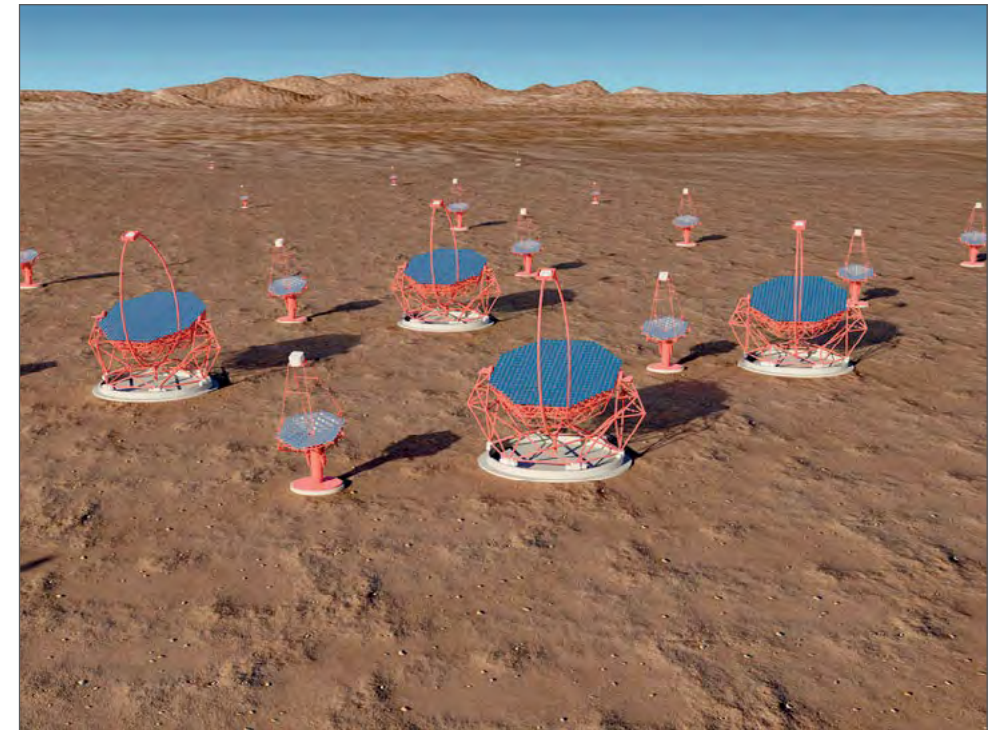


## High Energy Gamma-Rays from Universe

Radiation at gamma-ray energies differs fundamentally from that detected at lower energies. Energies of gamma rays of the order of GeV to TeV cannot conceivably be generated by thermal emission from hot celestial objects. Instead, we find that high-energy gamma-rays probe a “non-thermal” universe and objects with the concentration of large amounts of energy onto a single quantum of radiation. These gamma-rays can be generated when highly relativistic particles – accelerated for example in the gigantic shock waves of stellar explosions – collide with ambient gas, or interact with photons and magnetic fields. High-energy gamma-rays can also be produced by possible decays of heavy particles such as the hypothetical dark matter particles or cosmic strings, both relics which might be left over from the Big Bang. Therefore, gamma-rays also provide a window onto the discovery of the nature and constituents of dark matter. The Cherenkov Telescope Array (see Fig. 3) will be the new generation observatory of (very) high-energy gamma-rays and as such it will allow discovery of a large number of new astrophysical sources of gamma-rays and the determination of their characteristics [8]. will address fundamental questions related to dark matter as well.



**Fig. 4:** All-sky cameras deployed around the world by the group from the Institute. Eight cameras were successfully deployed at remote sites in the CTA site selection campaign.



**Fig. 3:** Artist's concept of one of the possible configuration of the CTA array. The CTA Observatory will comprise several (most likely 3) different sizes of telescopes deployed across ten square kilometers in case of the southern site (one square kilometers at the northern site).

In 2011 the Astroparticle Physics Group of the institute joined the CTA Consortium and initiated a substantial increase of the Czech involvement in CTA. Within a few months the group from the institute had become widely recognized and highly visible in several CTA work packages. The intensive involvement of the institute in the CTA Observatory would be a natural continuation of current involvement in the Pierre Auger Observatory both from the scientific as well as from the technological point of view. Currently, the department is responsible for analysis of satellite images for characterization of properties of the proposed sites of CTA location. Olomouc laboratory developed all sky cameras (see Fig. 4) which monitor cloudiness above eight candidate sites [9]. The CTA mirror prototypes and mirror samples are extensively tested in the institute [10]. Based on the experience from the Pierre Auger Observatory, we are also designing a robotic telescope to be used as monitoring instrument of the immediate observational conditions above the CTA Observatory.



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## Department of Detector Development and Data Processing

The personnel of the department consists of physicists, electro-engineers, electro-mechanical technicians and computer specialists. The working teams are contributing to several research projects of the division, some of them in collaboration with other departments. In detector laboratories we can setup and test detectors in clean rooms at special atmospheres or temperatures. Our engineers and technicians in the electronics laboratory developed specialized power supplies, LED drivers, amplifiers and special devices. We have a small mechanical workshop for finishing of electronics designs and other detector developments. We also develop, support and maintain computing and networking services.

The department has contributed to the following international experiments and projects: ATLAS/TILECAL at CERN; D0 and NOvA at Fermilab; H1 at DESY and CALICE – EUDET/AIDA.

The department has expertise in designing hadron and electromagnetic calorimeters, silicon detectors, electronics and special power supplies. Further it provides the first line computing user support for our department, runs computing resources and supports the Windows and Unix personal computers and computer network for its members. It also offers software distribution services and experimental equipment repairs to the whole institute.

## Research Highlights

### The D0 Experiment

The D0 experiment is an antiproton–proton experiment at the Tevatron accelerator at Fermilab, close to Chicago (USA). We joined the experiment in 1989 for a Run II upgrade, that took place after the discovery, together with the competing Tevatron experiment CDF, of the top quark in Run I. The upgrade was designed to enable detailed measurement of the top quark properties and we contributed to it with the work of our physicists and technicians both in Prague and in Fermilab. After the Run II upgrade the detector had been equipped with a micro-strip silicon tracker with a magnetic field of 2 T, precise calorimeter and hermetic fine grain muon system.

The Tevatron accelerator delivered the highest colliding beams energy of that time,  $1 + 1$  TeV, and the detector produced number of high precision results in b-physics,

top-quark physics, new phenomena and also discoveries such as single top quark production. The Tevatron operation was stopped in 2011, at the time when LHC was steadily running and taking data. The D0 experiment published nearly 500 papers, of which we are co-authors of 320 [1,2].

Our main contribution was the study of jet production and calibration that provides a basis for many of the precise measurements. In addition, measurement of mass and production channels of the top quark was carried out. Moreover, the computing farm in the Institute of Physics delivered up to 20 % of the computing capacity to the experiment in the final years. We also took part in experimental management. The successful collaboration was supported by the Ministry of Education, Youth and Sports of the Czech Republic through INGO II program grants.

### The NOvA Experiment

We joined the NOvA experiment in 2011 and this formed our main intensity frontier experiment at Fermilab. NOvA, Fermilab's new flagship neutrino oscillation experiment, has recorded its first neutrinos and is now poised to make precision measurements of electron-neutrino ( $\nu_e$ ) appearance and muon-neutrino ( $\nu_\mu$ ) disappearance. These data will help to unravel the remaining unknowns in our understanding of neutrino masses and mixing. NOvA will use two detectors to measure oscillation probabilities in Fermilab's NuMI (Neutrinos at the Main Injector) muon neutrino beam. When neutrinos

travel the 810 km between Fermilab and Ash River (Fig. 2) in Minnesota, through the crust of the Earth, scattering of  $\nu_e$  on atomic electrons can either enhance or suppress the oscillation probability, depending on the mass hierarchy. The effect is opposite in neutrinos compared to antineutrinos, so by comparing the oscillation probability measured in neutrinos to that measured with antineutrinos, NOvA can determine the mass hierarchy, resolve the nature of mass eigenstate  $\nu_3$ , and begin the study of CP violation in neutrinos.

In addition to an intense beam, NOvA also requires a massive Far Detector and a functionally identical Near Detector. Like all neutrino detectors, the NOvA detector must be big to overcome the small size of the neutrino interaction cross-section and the 810 km distance from the neutrino source. Being big, however, is not enough; the detector must also be highly segmented to prevent the numerous cosmic rays that cross the detector from interfering with neutrino events from Fermilab.

The NOvA detectors (Fig. 3) are a unique solution to the particular challenges of observing  $\nu_e$  appearance using the NuMI neutrino beam line. The NOvA Far Detector is a 14,000 ton detector, using 9000 tons of liquid scintillator – the largest quantity of liquid scintillator ever produced for a physics experiment – to record the tracks of charged particles. The scintillator is contained in a  $15.6 \times 15.6 \times 64$  m<sup>3</sup>, 5,000 ton PVC structure constructed from modules. In addition to containing the scintillator, the PVC structure segments the detector into  $4 \text{ cm} \times 6 \text{ cm} \times 15.6 \text{ m}$  channels. Light produced in these channels by the charged particles that traverse them bounces 10x on average before it is captured in a wavelength shifting fibre. The Prague laboratory, with experience in avalanche photo diodes has contributed to the construction, commissioning and running of the experiment. Our colleague has fulfilled the responsible role of a run coordinator of the NOvA experiment at Fermilab since 2013. We have also enabled our computing capacities in the Institute of Physics in Prague as an OSG site to be able to simply deliver computing capacities to NOvA.



Fig. 2: NOvA long baseline experiment spanning the distance between Fermilab and Ash River

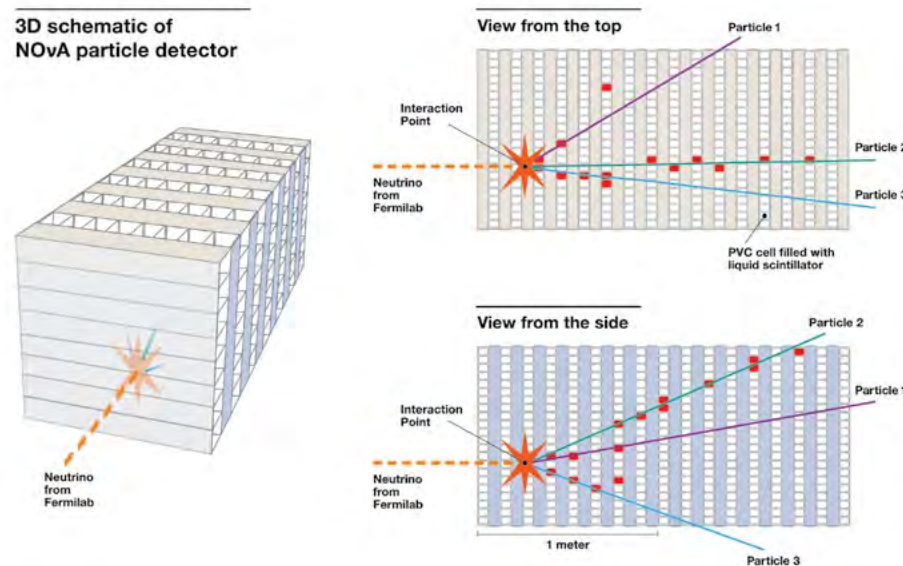


Fig. 1: Schematics of the NOvA experiment



## CALICE – EUDET/AIDA

The research and development project aimed at significant improvement in the energy resolution of jets concentrates on imaging calorimetry. We participate in the CALICE collaboration in two aspects: the compact electromagnetic SiW calorimeter and the scintillator tile calorimeter with SiPM readout. In the year 2010 the test beam campaign of the calorimeter prototypes which started in 2006 and exploited particle beams at DESY, CERN and Fermilab was completed [5]. The results from the tests are frequently published and the second generation of calorimeter prototypes is now under construction [3–4]. In Europe this research was also supported by EU grants for the projects EUDET (until 2010) and AIDA (2011–2015). This research and development project is mainly oriented to the energy range of the future linear colliders but several spinouts have found applications both in and outside particle physics, e.g. the SiPMs, first extensively used in the CALICE tile calorimeter prototype and upgrades of CMS and COMPASS calorimeters, are now used in the proton computed tomography and positron emission tomography.



Fig. 3: J. Zalesak from the Institute of Physics during the work on NOvA detectors

## ATLAS/TILECAL

The researchers from the department are actively involved in the ATLAS Collaboration at CERN. Their activities are mostly connected to the Tilecal hadronic calorimeter, and are realized in close collaboration with the scientists from the Department of Experimental Particle Physics. Therefore, more thorough description of these activities

is presented between research highlights of the Department of Experimental Particle Physics on page 56.

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## Department of Experimental Particle Physics

Research activities of the department are focused on particle physics experiments realized in international collaboration with major world laboratories, in particular CERN in Geneva (Switzerland) and FNAL in Batavia (USA). We are engaged in physical analysis of experimental data as well as in the preparation of new experiments, their development, construction, and subsequent operation and maintenance of realized experimental devices. We also participate in research programs to develop new types of detectors and experimental techniques.

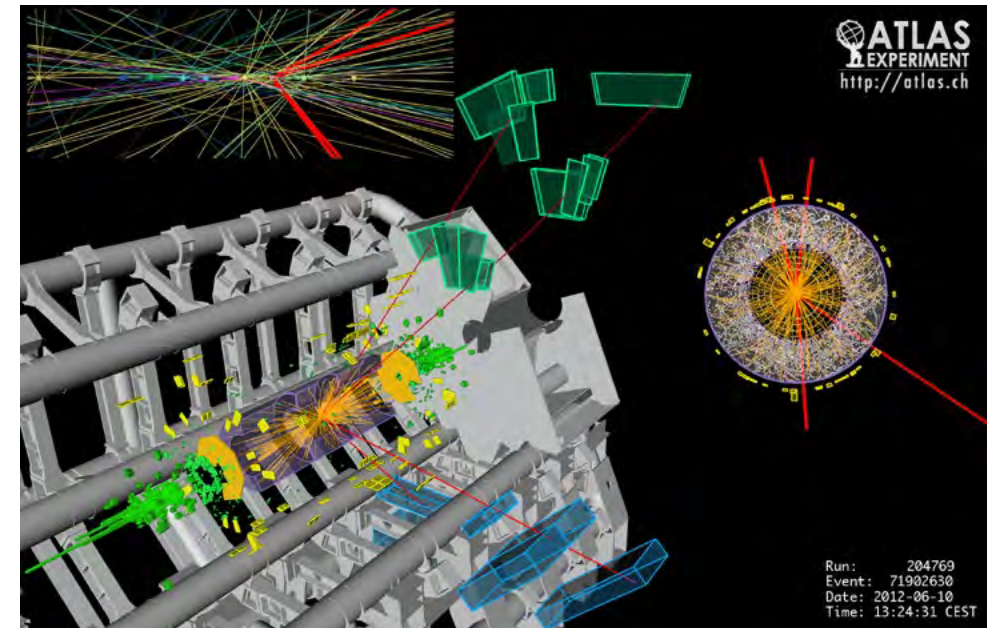
Our scientists and engineers contributed in the past to the construction, operation, and analysis of the data in several international experiments, such as the H1 experiment at HERA in Hamburg (Germany), the former experiment DELPHI at the electron-positron accelerator LEP at CERN, the experiment D0 at FNAL, and the current experiment ATLAS at Large Hadron Collider (LHC) at CERN. The major activity of the department is naturally focused on ATLAS in order to exploit the scientific opportunities offered by this unique experimental device.

As far as development of new detectors is concerned, the department is active in developing radiation hard semiconductor detectors for ATLAS, pixel detectors for the MediPix project, various voltage supplies for calorimeters and tracking semiconductor detectors, and silicon pad detectors for the electromagnetic calorimeter of the CALICE project. These research activities are carried out in close collaboration with the following international projects: AIDA (Advanced European Infrastructures for Detectors and Accelerators), RD50 (Radiation hard semiconductor devices for very high luminosity colliders), EUDET (Detector research and development towards the International Linear Collider), CALICE (High granular calorimetry for future particle physics experiments), MediPix (Family of photon counting pixel detectors).

### Research Highlights

#### Experiment ATLAS at CERN

The Institute of Physics is a founding member of the ATLAS Collaboration. In the years 1992–2008, this group of about 3000 scientists from more than 170 laboratories and universities across the world has built the detector, ATLAS, one of the most complex scientific instruments ever constructed by mankind. ATLAS, together with its “sibling” and competitor CMS, are the two largest LHC experiments, designed to explore the discovery potential of LHC in proton-proton collisions.



**Fig. 1:** Event display of a proton-proton collision recorded by the experiment ATLAS. Scientists in this event identified possible candidate for Higgs boson decaying via two intermediate Z bosons into four muons (long red lines).

Our researchers contributed mainly to the design and construction of the inner tracking detector and hadronic calorimeter Tilecal. New laboratories have been established on the premises of the institute for testing semiconductor sensors and assembling Tilecal modules. Close cooperation with industry led in the past to the conclusion of contracts of Czech companies with CERN, resulting in deliveries of pixel sensors and various high and low voltage power supplies. To increase the impact of Czech scientists in the ATLAS Collaboration, the Institute of Physics closely coordinates its activities with Charles University in Prague, the Czech Technical University in Prague, and Palacký University in Olomouc. Participation of these four institutions in ATLAS has been supported since 1996 through various programs of Ministry of Education, and Ministry of Industry and Trade of the Czech Republic.

Currently, there are four active ATLAS groups in the institute: the tracking group, calorimeter group, forward physics group and general physics group. The tracking group is responsible for operation, maintenance, and upgrades of the inner tracking detector. The calorimeter group is responsible for the maintenance and operation of Tilecal, mainly its low voltage power supplies. The forward physics group is playing an active role in proposed project of new forward proton detectors, AFP. The group has been involved in the process of defining the physics program for the project and it is also



contributing to the management, design and construction of the first prototypes. Activities of the physics group are mostly focused on the analysis of collected data.

Years 2009–2012 were significant as the first long data taking period at the LHC. The successful run was crowned by the discovery of the Higgs boson, announced in July 2012 [1], by ATLAS and CMS. The discovery was confirmed a year later after analyzing more data collected during 2012 at slightly higher energy. The Nobel Prize in Physics 2013 was awarded to F. Englert and P. Higgs, and the crucial role played by LHC experiments was acknowledged in the Nobel Committee's citation:

*"[for] the theoretical discovery of a mechanism that contributes to our understanding of the origin of mass of subatomic particles, and which recently was confirmed through the discovery of the predicted fundamental particle, by the ATLAS and CMS experiments at CERN Large Hadron Collider."*

Smooth operation of detectors developed and constructed in cooperation with our institute, the inner tracker and the hadronic calorimeter, was essential for the discovery. The LHC has been undergoing a major upgrade in 2013–2015. Starting from 2015, the machine will provide proton–proton collisions close to the designed energy of  $\sqrt{s} = 14$  TeV. The plan is to reach in the following seven years ten times higher luminosity (a measure of the number of collisions) than in the first run. The ATLAS detector



**Fig. 2:** *Insertable B-Layer – new layer of pixel detectors was added to the ATLAS inner tracker detector during the last LHC shutdown. Institute of Physics contributed to the development, construction and installation of this device.*

has to be prepared for this new harsh environment. The major upgrade concerns the tracking detector. A new insertable layer of pixel detectors was installed in 2014 close to the accelerator's beam pipe in order to provide better recognition of displaced secondary vertices coming from the decays of hadrons containing bottom quark. The Institute of Physics participated in the development and testing of pixel detectors for the project, and our researchers are responsible for the operational tasks during the installation and following commissioning phase of the insertable layer.



**Fig. 3:** *M. Tomášek and J. Mládek from Institute of Physics during the work on the pixel detector in the ATLAS experimental hall*

The tracking group is also involved in several CERN research and development projects. The aim of the project RD50 is to develop radiation hard semiconductor devices for future very high luminosity colliders. RD53 develops infrastructure for advanced readout microchips. The group is also active in testing new strip detectors for the upgrade of the ATLAS tracker, foreseen to operate after high luminosity upgrade of LHC in 2024.

Data collected by ATLAS in the years 2009–2012 contain valuable scientific information. The collaboration published or submitted more than 260 papers since 2010. Our researchers contributed to this effort in the following areas: diffractive and soft physics, jet physics, di-boson production and physics of bottom and top quarks [2–6]. The group is dynamic, having many undergraduate students, several doctoral stu-

dents, post-doctors and and young fellows. Their work is highly regarded in ATLAS, for example one of our young fellows was leading the ATLAS Soft QCD Group between 2010–2012.

The group plays an important role in education and training as well. ATLAS represents a unique opportunity for Czech students to be involved in world class research activities even in the early stages of their curricula. Doctoral students can carry out their scientific research in international teams with renowned scientists. Technically oriented students benefit from the work with cutting edge technologies.

For the Institute of Physics, the participation in ATLAS experiment represents a unique possibility to contribute to the world-wide effort in the pursuit of fundamental laws that govern the behavior of the matter and universe around us. The hope is that with increased statistics and higher collision energy, the LHC experiments can reveal new unknown phenomena outside the framework of the current Standard Model of particle physics. That might help us to answer open questions about the origin of dark matter and dark energy. After all, current astronomical observations are telling us that the particles from the Standard Model constitute only about 4% of the universe.

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## Department of Particle Theory and Phenomenology

The activities of the department range from purely theoretical and formal topics within string theory, to the phenomenological aspects of real-world hadrons – strongly interacting particles. In fact, about half of the members of the department are actively involved in some of the major high-energy particle physics experiments at CERN (Atlas, Alice, Totem), that are covered in other parts of this booklet. Herein, we divide the description of the department's research into three highlighted areas: string field theory, quantum gravity and particle phenomenology in general.

## Research Highlights

### String Field Theory

One of the major research lines of the theory and phenomenology department since 2009 when Dr. Schnabl joined our institute has been the study of string field theory. String field theory is a particular approach to string theory, a highly mathematical theory which aims to unite the four fundamental forces of nature purely on the principles of mathematical beauty and quantum consistency. Vibrating modes of a given string correspond to various elementary particles, which in a proper quantum theory must give rise to quantum fields. The string field theory is a theory of such fields.

Quantum field theory is one of the most useful and universal tools in contemporary theoretical physics, and is not limited to high energy physics only. In general it becomes indispensable when we study collective phenomena (e.g., phase transitions) in a system with lots of degrees of freedom. Another example is the celebrated Higgs mechanism, which explains why, in the standard model of elementary particle physics, initially massless particles obtain mass.

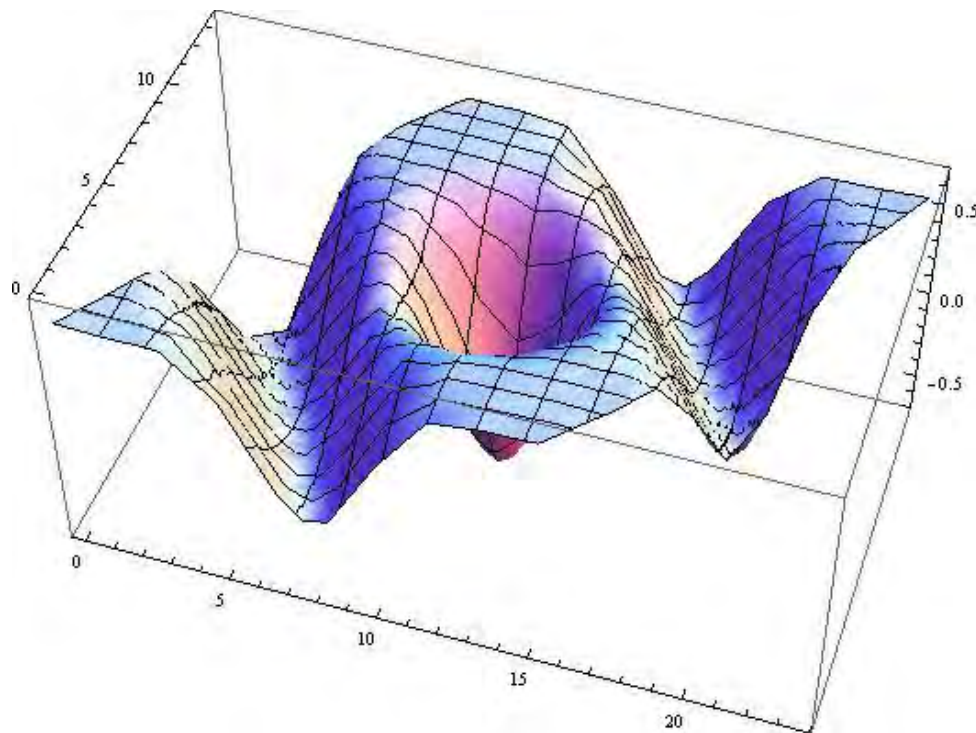
Open string field theory is in many respects very much like the gauge theory of the standard model. The counterpart of the Higgs field is called for historical reasons the tachyon field. The tachyon field in string field theory tends to condense in a wide variety of ways. Often the field condenses everywhere, except in the neighborhood of some hypersurfaces called D-branes. In the complementary world-sheet approach to string theory, the D-branes are described by a choice of conformal boundary conditions of the quantum two-dimensional conformal theory living on the string worldsheet.

The theory of conformal boundary conditions in two dimensions is not only important in string theory, it has very diverse applications in other branches of science: from study of quantum impurities in a one-dimensional system of condensed matter



to highly abstract concepts in pure mathematics. We have proposed that string field theory presents a novel, more powerful constraint for such boundary conditions and have shown how to actually turn classical solutions into proper boundary states [1]. The difficult part is now to construct these solutions explicitly.

The simplest solutions can be easily found numerically, as was already realized some time ago. In 2005 however, it was realized by Schnabl [2] that a solution describing spatially homogenous tachyon condensation can be found analytically. In 2009 with Erler they found a conceptually much simpler expression which then enabled lots of the subsequent progress. Then in 2011 Schnabl and Murata discovered a very simple general formula for the energy and the boundary state for this and other solutions, which raised the possibility for the existence of multiple D-brane solutions [3]. While most of these developments took place in the simplified bosonic string theory, Erler in 2013 succeeded in solving the analogous problem for the more realistic superstring theory [4].



**Fig. 1:** Profile of the tachyon field on the two-dimensional torus represented by the parallelogram. This particular configuration corresponds to a superposition of one-dimensional D1-brane and point-like D0-brane.

Inhomogenous, or background dependent solutions are much harder to find. In 2014 Kudrna, Rapčák and Schnabl presented a systematic approach, describing how to search numerically for such solutions [5]. Later that year Erler and Maccaferri took a major step towards analytic description of these, and we may witness rapid development in this area in the near future.

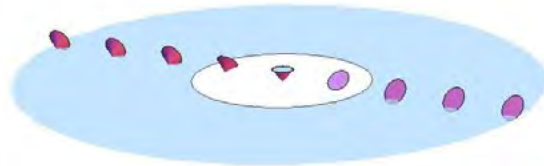
Besides these formal and interdisciplinary aspects of string field theory, there are important physical applications which we plan to address in the near future. To name just two: the physics of intersecting D-branes in string theory is tantalizingly close to the physics of the standard model, including the Higgs mechanism. Could the Higgs field be the stretched string tachyon? Another intriguing possibility to relate the string field theory to the real world is via the physics of the early universe inflationary period.

## Quantum Gravity

The 20<sup>th</sup> century saw the emergence of two of the most successful theories in physics: Einstein's theory of general relativity describing gravitational force, and quantum mechanics, describing the peculiar behavior of particles on the smallest scales. Under closer scrutiny, these theories turn out to be incompatible: general relativity seems to have insurmountable problems when viewed as a quantum theory of particles. The aim of quantum gravity is to reconcile general relativity with quantum mechanics. In string theory, which is widely believed to be a consistent quantum gravity theory, the conundrum is resolved by replacing particles as the smallest constituents of matter with tiny vibrating strings. An important insight which came out of string theory, but which may be more generally valid, is the concept of holography: quantum gravity can be reformulated as a quantum mechanical theory without gravity which lives on a "holographic screen", a surface of one lower dimension. The research in our group aims to use tools from string theory and holography to address open questions in quantum gravity. In the period 2010–2014 we have focused on three main problems.

### Are Time Machines Unphysical?

In 1949, mathematician Kurt Gödel demonstrated the mathematical possibility of time machines: solutions to Einstein's equations of general relativity representing universes where observers can travel back in time to an earlier point in their history. We say that such a universe contains closed time like curves (see Fig. 2). Time machines present physicists with seemingly unresolvable paradoxes such as traveling back in time to murder one's own grandfather. Basically, a time machine destroys the relation between cause and effect which allows us to formulate physical laws. Therefore, time machines are widely believed to be unphysical. This led Hawking to formulate his famous chronology protection conjecture in order to "make the universe safe for historians". Our interest in the chronology protection conjecture was sparked after we discovered that Gödel's universe also arises as a so-called "BPS solution" in certain theories of gravity, implying that it is more stable and well-behaved than we original-



**Fig. 2:** Left – Gödel and Einstein in the early 1950s. Right – space-time diagram of Gödel's time machine. For each observer we can draw a light-cone which contains events accessible in his future. The blue region contains closed timelike curves.

ly thought. We decided to study chronology protection using ideas from holography and asked the following question: suppose the universe contains a time machine, do we see any unphysical behavior in the quantum mechanical theory on the holographic screen? In the cases we have studied it indeed resulted in violation of a basic principle of quantum mechanics, unitarity [6]. Our investigations hence suggest that quantum mechanical unitarity forbids the construction of time machines in general.

### The Internal Structure of Black Holes

Einstein's theory of general relativity was long known to predict the existence of black holes, the end products of gravitational collapse from which not even light can escape. Naively, black holes seem to be rather simple objects which are completely determined by three parameters: mass, angular momentum and charge. However, it was argued by Bekenstein and Hawking in the 1970s that black holes behave like thermodynamic systems possessing a temperature and an entropy, suggesting instead that a black hole can be in any of a gigantic number of microscopic configurations which are indistinguishable for the outside observer. A quantum theory of gravity should give a description of these so-called microstates and explain the origin of the black hole temperature and entropy. One of the main successes of string theory is that it passed this test, as was shown by Strominger and Vafa. The concept of holography was crucial for this, as the microstates were identified and counted in the quantum mechanical theory living on a holographic screen.

This exciting result immediately raised the question of whether we can also identify the microstates in the gravity theory, not just on the holographic screen, and study their geometry and physical properties. As stressed by Mathur, the standard ideas of holography suggest that this should be possible and that gravity theory should contain smooth solutions which correspond to the microstates. In Mathur's picture the naive



**Fig. 3:** In Mathur's fuzzball picture of black holes, the singular black hole (left) is replaced by a smooth geometry with internal structure (right). (Figure courtesy of Nick Warner.)

singular black hole geometry has to be replaced by a smooth microstate geometry with some internal structure, a so-called "fuzzball" (see Fig. 3).

The program of constructing these microstate geometries has so far succeeded only for the simplest "small" black holes, where the theoretical description is however not completely reliable. For the "large" black holes, where we do have a reliable description, the microstate geometries have not yet been found yet. In our work, we have focused on the black hole deconstruction proposal of Denef et al.. The main technical hurdle was that the proposed solutions live in a branch of the theory which is not much studied, requiring us to develop new techniques to construct them [7]. After much hard work we were able to construct the simplest microstate geometries, albeit so far not analytically but only in a perturbative expansion [8].

### Holography for Higher Spin Gravity

The last topic we have studied is perhaps a little more abstract but nevertheless very exciting for us, as it is part of a field which saw major progress in the last few years. The idea is to construct holographic quantum gravity theories where the quantum mechanical theory on the holographic screen is as simple as possible. Such theories seem the ideal setup to address the thorniest questions in quantum gravity such as the black hole information paradox, the nature of the cosmological big bang singularity and so on.

It turns out that the simplest holographic theories do not only describe gravity but also contain exotic massless "higher spin" particles which have not been observed in nature. Theories containing these hypothetical particles were constructed only fairly recently by Vasiliev. They are not only of academic interest. The higher spin theories may be relevant to early universe physics.

Our interest in this subject was sparked in 2011 when Gaberdiel and Gopakumar proposed a very concrete example of a simple holographic theory. Our research has focused on resolving a puzzle in the Gaberdiel-Gopakumar proposal: the holographic minimal model theory contains a class of light excitations which do not seem to be present in the higher spin theory. We were able to show that, at least in some region



of parameter space, these excitations do appear in the higher spin theory as previously unknown smooth classical solutions [9]. Since then we have accumulated further evidence that these solutions have the correct charges and symmetry properties to be identified with the minimal model excitations [10].

## Phenomenology

### The Three-Dimensional Quark–Gluon Structure of the Nucleon

Over the past 40 years an understanding of nucleons in terms of partons (i.e., quarks and gluons) has gradually and successfully developed. Much has been learned about the nucleon in terms of its “one-dimensional” parton structure, relevant when partons are assumed to move co-linearly with their parent nucleon, and encoded in so-called parton distribution functions. In the last few years theoretical breakthroughs have extended this simple picture, leading to new concepts like the “Generalized Parton Distributions” and the “Transverse Momentum Dependent parton distributions”. These concepts are used to address long-standing questions concerning the motion of quarks and gluons inside the nucleon: their orbital motion, their spin and their spatial distribution. We contribute to this program by studying these questions in the framework of the covariant parton model [11] which we developed earlier.

### Interaction of Ultra-Relativistic Ions in the LHC Experiment ALICE

Study of heavy ion collisions at ultra-high energies represents a hot topic in contemporary nuclear and particle physics. A fundamental motivation for this study is to verify the prediction of Quantum Chromodynamics which implies that at very high temperatures and very high densities of nuclear matter, quarks and gluons should exist unconfined, in a new state of matter known as quark–gluon plasma. We believe that the entire universe was in this state for a short moment just after the Big Bang. Similar conditions are created in the volume of colliding nuclei in the ALICE experiment at LHC. Our group participates in analysis and Monte-Carlo simulations of some processes in the ALICE experiment (calculations are performed on our computer farm Golias). It also takes part in the maintenance and operation of the PHOS spectrometer, an important ALICE subdetector.

### TOTEM Experiment

The TOTEM experiment at the LHC at CERN has been devoted mainly to the detection of proton–proton collisions in which one or both protons survive the corresponding collision. Dedicated LHC magnet settings allowed measurement of collisions where no new particles are produced and the two colliding protons just slightly change direction (elastic scattering) at very low scattering angles. It has been found that a corresponding distribution of elastic momentum transfer differential cross section has

similar structure as at lower energies. The analysis of elastic scattering data gave the following values of integrated elastic cross sections: for the energy of 7 TeV the value of  $(25.4 \pm 1.1)$  mb [12], for 8 TeV the value of  $(27.1 \pm 1.4)$  mb [13]. Assuming the validity of the optical theorem the value of total cross section has been established to be  $(98.6 \pm 2.2)$  mb at the energy of 7 TeV and to be  $(101.7 \pm 2.9)$  mb at the energy of 8 TeV. Scientists from our group proposed a description of Coulomb–hadronic interference based on the eikonal model and optical theorem, which has also been used in the analysis. They are also developing a new model of elastic proton–proton collisions.

### Perturbative Expansion in Quantum Chromodynamics

The perturbative expansion in quantum chromodynamics is famously divergent, so one has to resort to clever summation methods. Using the technique of conformal mapping of the Borel plane, we defined a set of new expansion functions that resemble the expanded correlator and share the same singularity at zero coupling [14]. We tested the optimized series on non-strange hadronic decay of the  $\tau$ -lepton. While our optimized expansions exhibit stable numerical results in all computed orders (up to the 18<sup>th</sup> order), the standard series in powers of  $\alpha_s$  exhibits violent oscillations from the 6<sup>th</sup> or 9<sup>th</sup> order up to all higher computed orders.

### Anomalous couplings of gauge bosons

We studied various possible anomalous couplings of gauge bosons and how they would appear at the LHC with feasible future upgrades of today’s experiments [15]. Forward proton tagging devices, similar to TOTEM described above, can select events in which light is emitted off the scattered protons, allowing precise measurements of various final states produced via two-photon exchanges. This novel technique may lead to much better constraints of anomalous gauge boson couplings than those obtained with conventional methods.

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Institute of Physics  
The Czech Academy  
of Sciences

Division of Condensed  
Matter Physics



Research activities of the Division of Condensed Matter Physics focus on experimental and theoretical investigation of solids, particularly their mechanical, magnetic and dielectric properties. We are searching for new phenomena, which can potentially result in new useful material properties and functionalities to be used in novel engineering applications. For this purpose we prepare and characterize a range of model materials, such as single crystals with low dislocation density, bulk Heusler alloys with tailored physical properties, CVD nanodiamond films and coatings; materials with controllable dielectric and ferroelectric properties, new liquid crystal phases and nanoparticles and nanocomposites consisting of particle assemblies. Theoretical research focusses microscopic properties of electrons in condensed systems having macroscopic consequences for measurable magnetic, electric and transport quantities. We try to improve properties of advanced structural metals by modifying their microstructures. Recently, new research directions towards multiferroic materials and functional ferroelastic materials, such as shape-memory alloys and smart composites with unique thermo (electro, magneto) mechanical properties were introduced. Another trend consists in the growth of oriented research focussing development of applications of functional materials and coatings in medical devices, actuators and smart structures. Recently we also got engaged in biophysics and biomaterials research.

The Division consists of six research departments:

- Department of Magnetic Nanosystems p. 71
- Department of Dielectrics p. 78
- Department of Advanced Structural Materials p. 88
- Department of Functional Materials p. 96
- Department of Condensed Matter Theory p. 104
- Department of Chemistry

We would also like to mention that within this Division two laboratories operate jointly with Charles University; the Joint Low Temperature Laboratory and the Joint Laboratory for Magnetic Studies. Other operating laboratories of the division are one for X-ray studies "ROTAN" and a new laboratory "FUNBIO" which hosts modern experimental facilities for characterization of surfaces between organic and inorganic materials.

## Department of Magnetic Nanosystems

The department was established in 2013 as an up-to-date successor of the Department of Magnetism and Low Temperatures. Nowadays, the main research topics include **Magnetic nanoparticles** for treatment and diagnosis of tumors (supported by the RP7 project MULTIFUN), **Graphene-based nanostructures** with controlled topography and synergy of enhanced Raman processes, **Giant anisotropy f-electron magnets**, and **Fundamentals of turbulence in liquid helium**. The department has strong links to Charles University in Prague through active involvement in education and participation in two joint laboratories – the **Joint Laboratory of Low Temperatures** and the **Joint Laboratory for Magnetic Studies** (see Figs. 1, 2), and takes part in operation of the helium liquefier and management of cryogenics. The research laboratories provide a unique combination of extreme environments (temperatures from mK to 1000 K, magnetic fields up to 14 T and hydrostatic pressures up to 2 GPa) for studies of transport, magnetic and elastic properties of solids by a variety of methods including Mössbauer and magneto-Raman spectroscopies.



**Fig. 1:** Apparatus for generation of quantum turbulence, Joint Laboratory of Low Temperatures

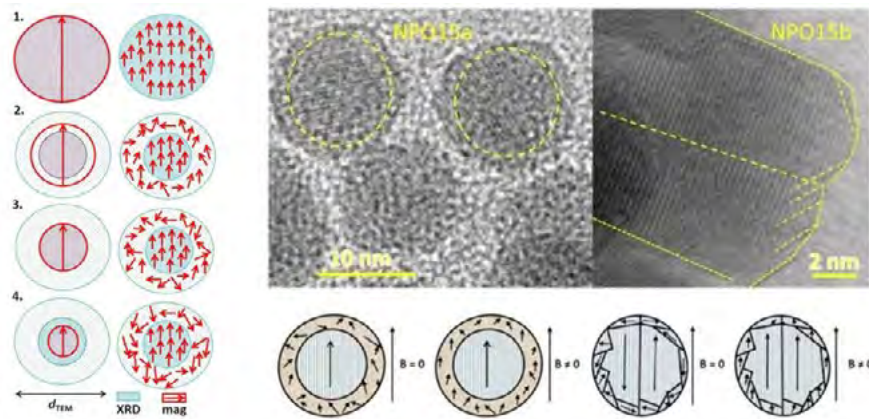


**Fig. 2:** Physical Properties Measurement Systems equipped with 9 T (A) and 14 T (B) superconducting coils, Joint Laboratory for Magnetic Studies

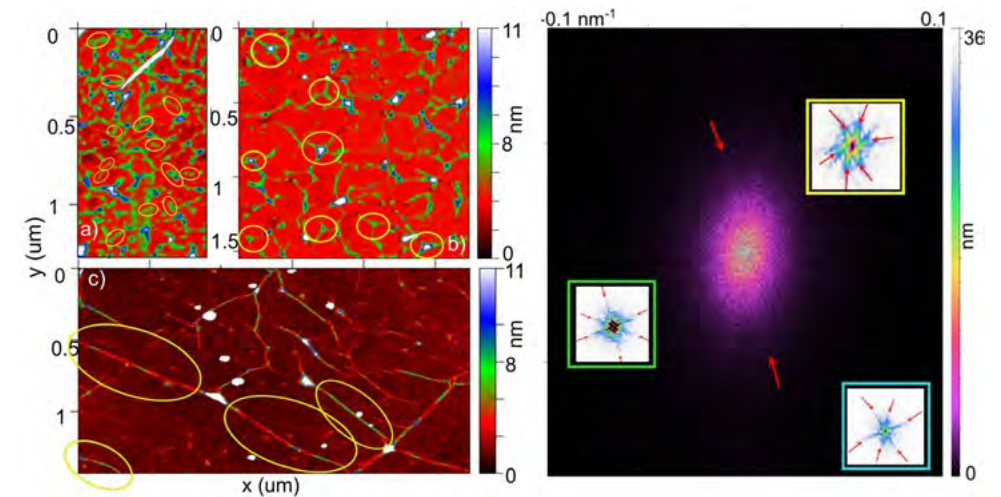
## Research Highlights

### Magnetic Nanoparticles & Nanocarbons

Nanoparticles of iron oxide are of enormous importance in biomedical applications due to their size-dependent magnetic properties and biocompatibility. Their exploitation has already been initiated as MRI contrast agents, hyperthermia mediators and drug carriers. One of emergent objectives of today's nanomedicine is to develop multimodal nanoparticles with simultaneous **therapeutic** and **diagnostic** abilities giving rise to the so-called **theragnosis**. However, design and tuning of particles for proposed applications requires deep understanding of their magnetic properties with respect to their internal crystallographic and spin structures (see Fig. 3), and mutual interactions in dense systems. Therefore, we focus on in-deep characterization of nanoparticles with impact on the limits of real systems including **surface spin canting** [1, 2], inter-particle interactions, size distribution and the collective response of nanoparticle ensembles [3, 4]. For reliable classification of the surface spin canting phenomena in iron oxide nanoparticles, we proposed to determine the evolution of the hyperfine field with respect to the applied magnetic field by using in-field Mössbauer spectroscopy in order to obtain information on the complex response of spins in individual sublattices. Finally, we have broken the myth that the spin canting is a general feature for all nanoparticles; it was recognized as negligible in highly crystalline particles with sizes larger than 6.5 nm.



**Fig. 3:** Illustration of the limiting cases of the internal structure of nanoparticles with particle size determined from transmission electron microscopy (TEM), X-ray diffraction (XRD) and magnetic measurements (mag). The large arrow represents the particle superspin, while the small arrows correspond to individual magnetic moments per unit cell. The figure on right represents TEM images of particles with identical TEM size, but very different XRD and magnetic sizes together with schematic response of the spin structure to the applied magnetic field. The core-shell particles (left) show huge SAR value in contrast to almost no heating effect of the later ones.



**Fig. 4:** Control of graphene topography by magnetic nanoparticles. Left – atomic force microscopy images of the single-layer graphene with three different types of wrinkles: (a) Short wrinkles formed between two individual particles. (b) Multiple wrinkles escaping from the central area. (c) Long-line wrinkles. Right – preferential orientation of wrinkles observed on the 2D FFT images of topographical images. The insets represent areas of discrete propagation of wrinkles.

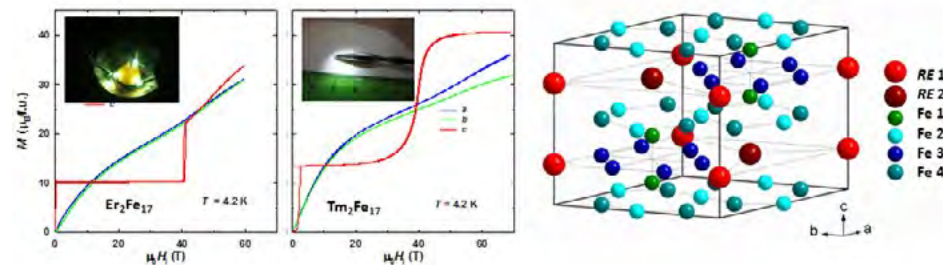
We also observed experimentally, that some level of **internal** particle spin and/or structural **disorder** is crucial for enhancement of the specific absorption rate (SAR) as a measure of the particle performance in magnetic fluid hyperthermia. The approach is a powerful tool for **prediction** of particle response in any application where the **functional** property depends on the **single particle anisotropy**.

Deep understanding of magnetic behavior of strongly interacting superparamagnets enabled us to decouple the response of residual metal catalyst in **single-wall carbon nanotubes** and significantly optimize their purification procedures leading to **extremely pure** samples for the first time [6, 7]. Recently, we succeeded in **control of topography** of **single-layer graphene** at nm scale by shaping the layer using a substrate decorated with monodisperse nanoparticles [8, 9] (see Fig. 4). Typical fingerprint of the wrinkles was clearly recognized in Raman spectra providing a general measure of wrinkling in graphene [8, 10]. We also succeeded in realization of tri-axial strain in graphene, which causes formation of Landau levels without presence of external magnetic fields. Our work thus demonstrated that the graphene topography can be both controlled and examined in a simple way, which provides a new impulse in strain-engineering of graphene-based nanodevices, site-specific enhancement of the graphene reactivity and investigation of fundamental phenomena related to local gauge fields.



## Highly Anisotropic *f*-electron Magnets

The rare earth (4*f*) intermetallic compounds with Fe or Co are famous as **extremely powerful permanent magnets** with exceptionally **high uniaxial magneto-crystalline anisotropy**. In  $R_2\text{Co}_{17}$  compounds (*R* is a rare-earth metal), the strongest interaction is the Co–Co exchange interaction which primarily determines their Curie temperature,  $T_C$ . The *R*–Co interaction, although much weaker than the Co–Co one, is of special importance since by this interaction the strongly anisotropic *R*-sublattice magnetization is coupled to the much less anisotropic Co-sublattice magnetization. The exchange interaction between the 4*f* and 3*d* electrons is usually represented by the molecular field, by which the *R*- and Co-sublattice moments are coupled. For the Co-rich *R*–Co compounds, the values for the molecular field are typically of the order of 100 T, so that large magnetic fields are needed to determine molecular field by induction of changes in the magnetic configurations of the two magnetic sublattices. Due to large magnetic anisotropy the study should be done on single crystals.  $\text{Er}_2\text{Co}_{17}$  and  $\text{Tm}_2\text{Co}_{17}$  (hexagonal crystal structure of the  $\text{Th}_2\text{Ni}_{17}$  type) are ferromagnets with rather similar magnetic properties [12, 13]. They have  $T_C = 1170$  K and spontaneous magnetic moment  $M_s = 10.1$  and  $13.4 \mu_B/\text{f.u.}$  for the Tm and Er compound, respectively, directed along the Co sublattice. In  $\text{Er}_2\text{Co}_{17}$ , the metamagnetic transition at 40 T

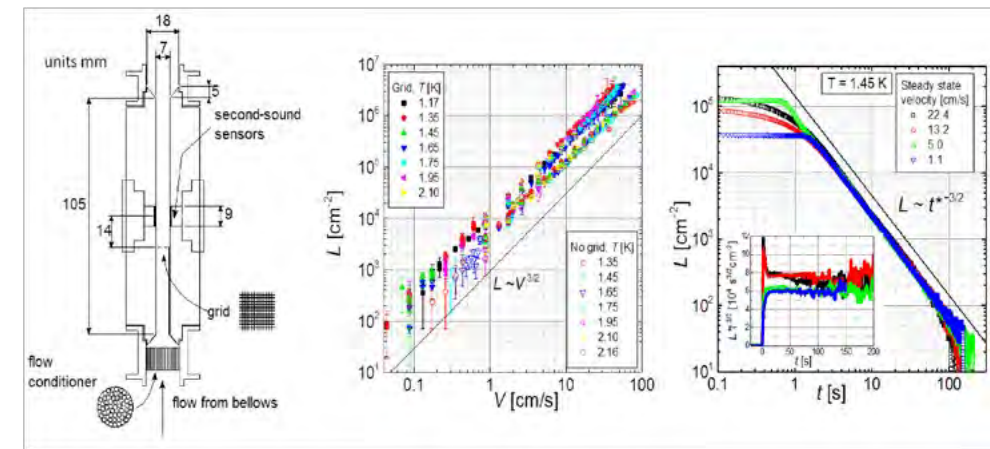


**Fig. 5:** High-field magnetization curves of the  $\text{Er}_2\text{Co}_{17}$  and  $\text{Tm}_2\text{Co}_{17}$  compounds with the pulsed magnetic field applied along the principal crystal axes. The unit cell of the  $R_2\text{Co}_{17}$  and  $R_2\text{Co}_{17}$  demonstrates packing of the 4*f* and 3*d* elements in the crystal structure. The insets show a typical crystal growth by the Czochralski method and the resulting ingot.

has been found in magnetic field applied along the *c*-axis (see Fig. 5). The transition is clearly of the first order and corresponds to sharp rotation of the Er sublattice by approx. 50 degrees with its further continuous alignment towards the collinear ferromagnet. We performed the high-field magnetization measurements of the  $\text{Tm}_2\text{Co}_{17}$  single crystal as well (see Fig. 5). Our most interesting finding is a large rise of magnetization in a field directed along the *c*-axis at  $\mu_0 H_{cr} = 39$  T. It is attributed to a direct ferri-to-ferromagnetic transformation by way of paramagnetic remagnetization of the Tm sublattice. This is a continuous process – no intermediate canted-spin phases occur and the sublattice moments remain collinear with the applied field. Thus, despite the similar-

ity of magnetic properties in fields below 20 T, the field-induced transitions in  $\text{Er}_2\text{Co}_{17}$  and  $\text{Tm}_2\text{Co}_{17}$  have completely different natures. The process of remagnetization of the *R*-sublattice without rotation of the magnetic moments is discovered for the first time.

The synergy of the properties of nanosized magnetite together with giant spin-orbit coupling and enormous magnetic anisotropy of *f*-electron systems stimulated original research on heterostructures composed of  $\text{UO}_2\text{-Fe}_3\text{O}_4$  thin films [8]. The exchange anisotropy between the antiferromagnetic and ferrimagnetic components originates a characteristic **exchange bias effect**, which is of fundamental importance for novel hard magnets, recording media, spin valve and tunneling devices.



**Fig. 6:** Apparatus for generation of the superfluid turbulence in  $^4\text{He}$  together with demonstration of scaling laws for the turbulence intensity,  $L$ .

## Quantum Turbulence

Quantum turbulence is the special type of turbulence of a quantum fluid, whose essential properties can only be explained by quantum physics. We work with liquid  $^4\text{He}$  at temperatures below 2 K, where the liquid exhibits the “**superfluid**” behavior. Among its properties is the ability to flow under certain conditions without viscosity, hence no energy dissipation. Superfluidity arises from the condensation of a large fraction of atoms in a single quantum-mechanical ground state, similarly to electron pairs in superconductors. Below the transition temperature, helium gradually becomes superfluid. Two components coexist in different ratios, a normal component, which has entropy and viscosity, and a superfluid component, which has zero entropy and viscosity. The turbulence possible in the normal component is similar to that of a classical fluid, but for the superfluid component, quantum mechanics imposes that a rotational motion is possible only by the generation of quasi one-dimensional vortices of Ångström width, called vortex lines. At small scales a turbulent superfluid is therefore a quantum,

discretized system, but at large scales the vortex lines can couple together normal and superfluid components resulting in an overall quasi-classical fluid. These quantum vortex lines are detectable in our experiments.

In our laboratory (<http://www.superfluid.cz/>) we generate superfluid turbulence similar to what engineers achieve in wind tunnels [14]. Our “tunnel” is a small channel (Fig. 6 left), where superfluid  $^4\text{He}$  is forced by a low temperature bellows. We measure the total length of vortex lines per unit volume ( $L$ ) by looking at how the propagation of sound through helium is modified by the presence of vortices. We are able to quantify the **scaling** of “**turbulence intensity**” ( $L$ ) with increasing flow speed over more than five orders of magnitude (Fig. 6 middle), which is far more than can be done in ordinary wind tunnels. Similarly, the decay over time of  $L$  can be followed for orders of magnitude (Fig. 6 right). This allows the extraction of very robust scaling laws [15]. We are finding that some of these laws are surprisingly the same as in classical fluids such as air or water, despite the quantum nature of helium. The emergence of universal behavior from very different systems points at fundamental laws of nature, and gives hope that studying quantum turbulence may become key to the **understanding of general turbulence**, still an open problem of classical physics, and extremely important for technical applications.

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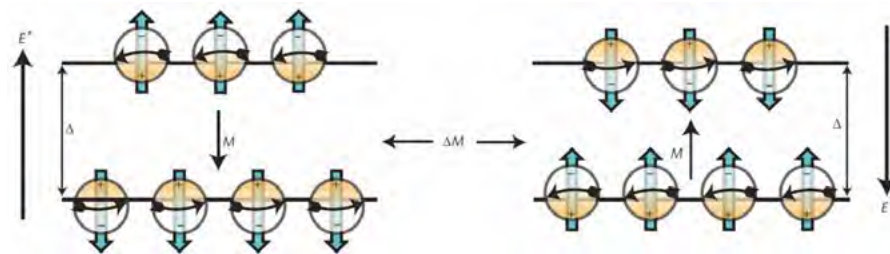
## Department of Dielectrics

The Department of Dielectrics is involved in detailed investigation of a range of advanced and model materials for which the frequency dependence of dielectric function can be probed by capacitance, waveguide or optical techniques. The main current research areas cover experimental and theoretical investigations of liquid crystals, ferroelectrics, multiferroics, piezoelectrics, nanocrystalline semiconductors and dielectric nanocomposites. The members of the department are involved in numerous national and international collaborative projects, mostly providing their expertise in dielectric, infrared, time-domain THz, Raman and neutron spectroscopy, but also in materials science and in state-of-the-art theoretical modelling. Typically, this research is aiming to elucidate the very nature of the interesting physical properties of the studied materials and, eventually, to derive structure–property relationships useful to change these properties in a desired way. Significant results were recently achieved for example in the studies of single-phase magnetoelectric multiferroics, ferroelectric domains and domain walls, as well as of new liquid crystals and artificial material structures with outstanding optical properties in the THz range.

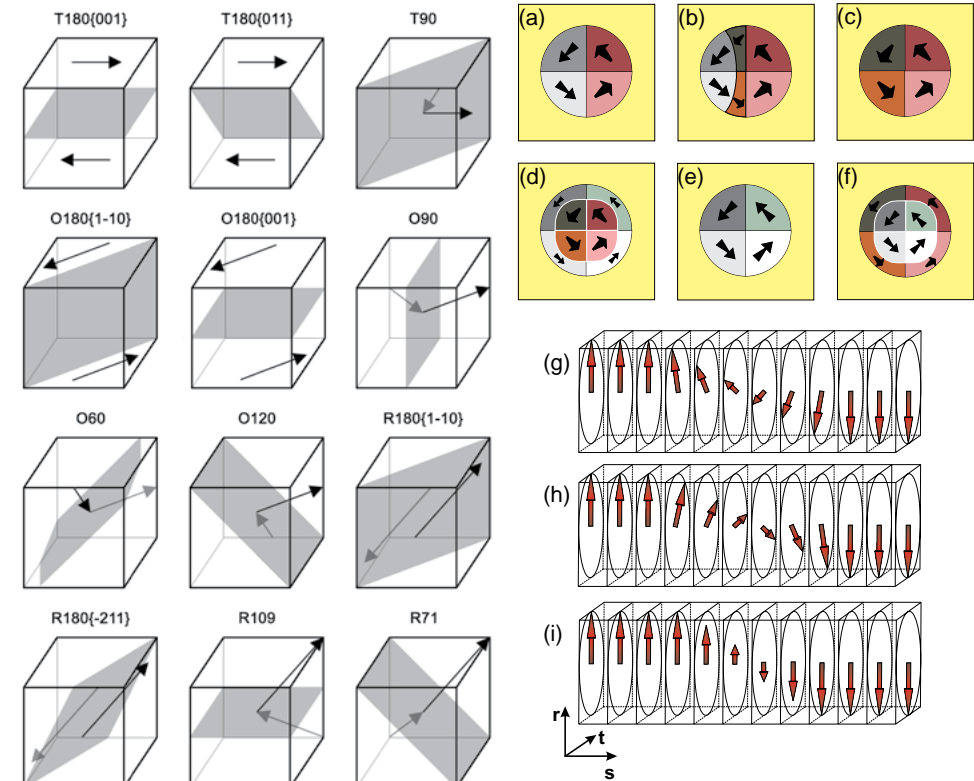
## Research Highlights

### Magnetoelectric Multiferroics

Magnetoelectric multiferroics are substances exhibiting magnetic and ferroelectric order simultaneously. These materials allow the control of magnetic or ferroelectric domains with electric or magnetic fields, respectively and raise the potential for applications in the technology of non-volatile memories. Unfortunately, the family of magnetoelectrics is not very numerous and most of the compounds show interesting properties only at low temperatures. Therefore intensive research is being carried out to



**Fig. 1:** Scheme of the principle of measurement of an electric dipole moment of the electron. Electric and magnetic moments of the electrons switch with switching of the electric field which leads to a change of the measured magnetization.



**Fig. 2:** Left: Set of mechanically compatible and electrically neutral domain walls of  $\text{BaTiO}_3$  for which the full analysis has been performed. Letter denominating the phase (T, O and R stand for tetragonal, orthorhombic and rhombohedral phases, resp.) is followed by an angle between the polarization vectors in adjacent domains (in degrees). Right: (a–f) Predicted stages of polarization switching in a ferroelectric nanorod, mediated by formation of exotic domain boundaries; (g–i) left- and right-hand ferroelectric Bloch wall and achiral Ising wall, respectively.

understand the very nature of the magneto–electric coupling and to induce the desired properties also at higher temperatures by preparation of suitably structured samples.

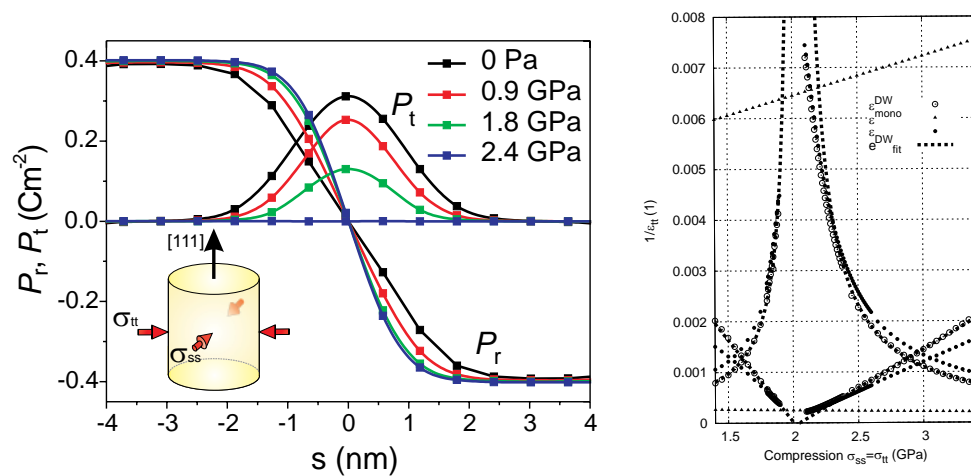
Cross-coupling between electric and magnetic subsystems is a subject that can be largely addressed by spectroscopic methods. For example, it has been suggested that large mechanical strain could be used in ultrathin films for preparation of new “artificial” multiferroics, and our team has experimentally proven that this scenario is valid in several materials. In particular, the originally antiferromagnetic and paraelectric  $\text{EuTiO}_3$  material changes to a strong ferromagnet and ferroelectric due to a strong spin–lattice coupling. Such a system should exhibit a strong magnetoelectric coupling which can be used in future memories [1]. It has been also suggested that a strong in-

ternal electric field in multiferroic  $\text{Eu}_{0.5}\text{Ba}_{0.5}\text{TiO}_3$  could be used for the search of permanent electric dipole moment (EDM) of the electron. According to the standard model of particle physics, its value should be of the order of  $10^{-40}$  e.cm. However, new theories of elementary particles propose an EDM of electrons of 8 or 12 orders of magnitude larger than the standard model. The physicists have been trying to measure the EDM of electrons for at least 40 years: they could reach a sensitivity of about  $10^{-27}$  e.cm. It has been shown [2] that in multiferroic  $\text{Eu}_{0.5}\text{Ba}_{0.5}\text{TiO}_3$  the sensitivity for such measurements should be an order of magnitude higher because of a strong internal electric field in the compound. Successful determination of the EDM value would enable the proof and specification of new theories going beyond the standard model of particle physics.

### Domain Boundaries: Ideal Two-Dimensional Nanoscale Model Objects

Miniaturization of electronic devices and the development of nanoscale characterization methods also drives new interest in ferroelectric domain boundaries. They can be viewed as intrinsic, about 1 nm-thick nano-objects, with their functional properties and on the top of this they can be created, annihilated, and moved by external electromechanical stimuli. However, theoretical studies are highly desirable to guide, challenging experimental efforts. Most efforts in our department were focused on the computer-aided predictions of domain-structure and domain-boundary properties of a model ferroelectric system  $\text{BaTiO}_3$ , relying on a specific Ginzburg–Landau–Devonshire-type phenomenological model.

An important milestone in this research was our systematic analysis of the properties of all mechanically compatible and electrically neutral domain walls in tetragonal, orthorhombic, and rhombohedral phases of the ferroelectric  $\text{BaTiO}_3$ . This work offered to the scientific community, the first explicit example of the complexity of pos-



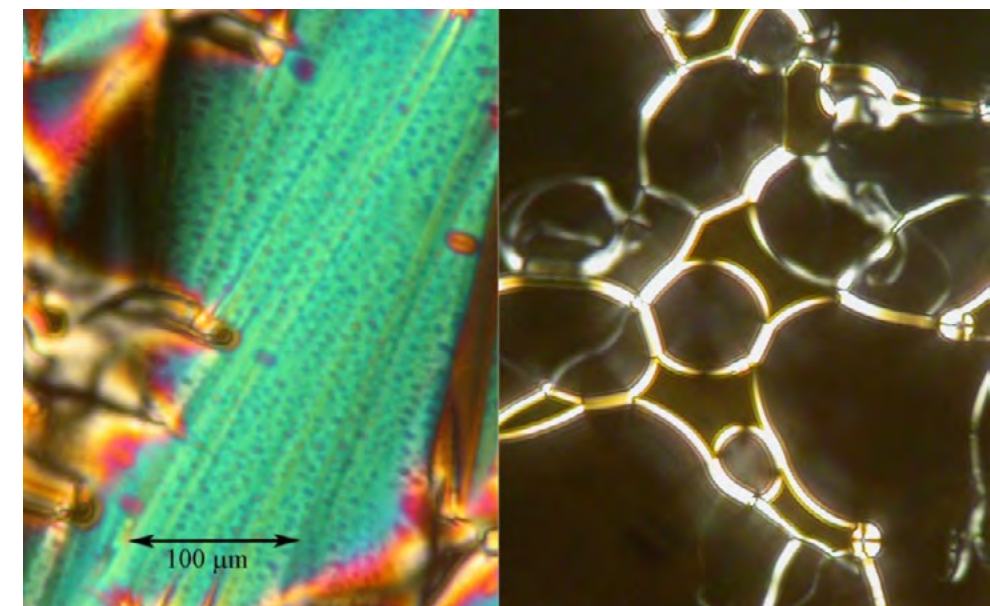
**Fig. 3:** Transition from Bloch wall to Ising wall. Left: vanishing of Bloch component of polarization. Right: Dielectric permittivity versus mechanical pressure.

sible domain wall species within a single material [3]. Even more exotic domain walls were found in ferroelectric nanorods [4]. Most interestingly, our calculations revealed that some domain walls resemble the chiral Bloch walls known from magnetism [3].

Ferroelectric Bloch walls are now the subject of numerous in-house and worldwide follow-up studies. For example, our computer simulations were used to study details of a chirality-breaking phase transition within the domain wall itself that leads to a bistable polar state, confined at a nanometer scale [5]. Divergent increase of the dielectric permittivity in the vicinity of this transition has also been confirmed in our work [6]. Results were later confirmed by standard ab-initio quantum-mechanical calculations [7].

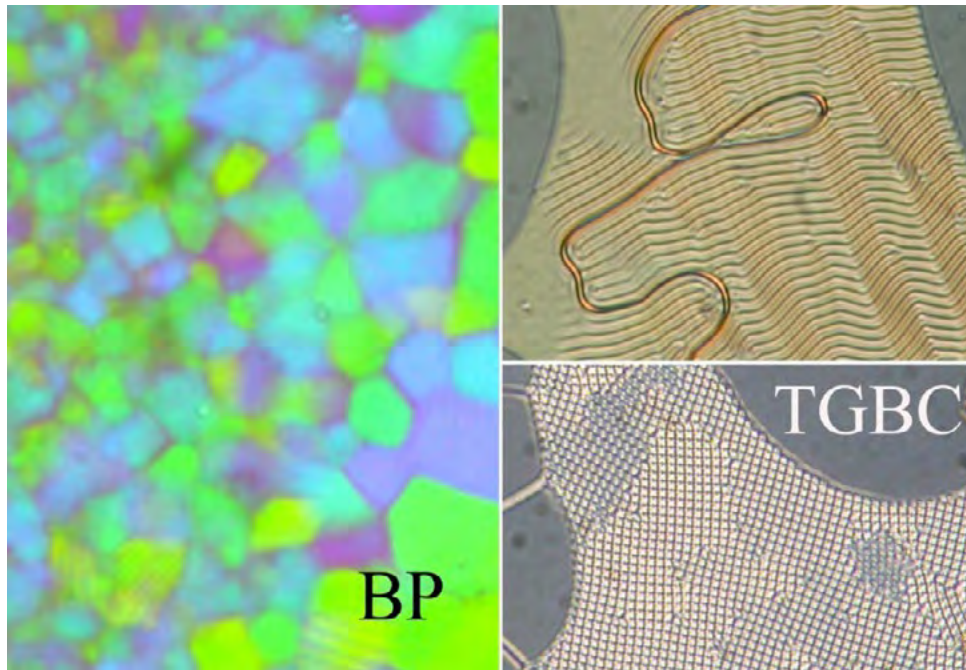
### Search for New Liquid Crystalline Materials

Formation of liquid crystalline phases is based on self-assembly of anisotropic organic molecules. Liquid crystals appear to be perfect candidates for formation of new multifunctional and composite systems. The Department is extensively involved in the design and study of new types of liquid crystalline systems. An example of a novel type of hybrid nanocomposite studied in department is a mixture of maghemite nanoparticles with a chiral liquid crystalline compound. This nanocomposite system exhibits ferroelectricity as well superparamagnetic properties. In the prepared material, a sizable influence of the magnetic field on its ferroelectric properties could be demonstrated [8].



**Fig. 4:** Texture of the smectic liquid-crystalline phase for two different nanocomposites with magnetic nanoparticles.



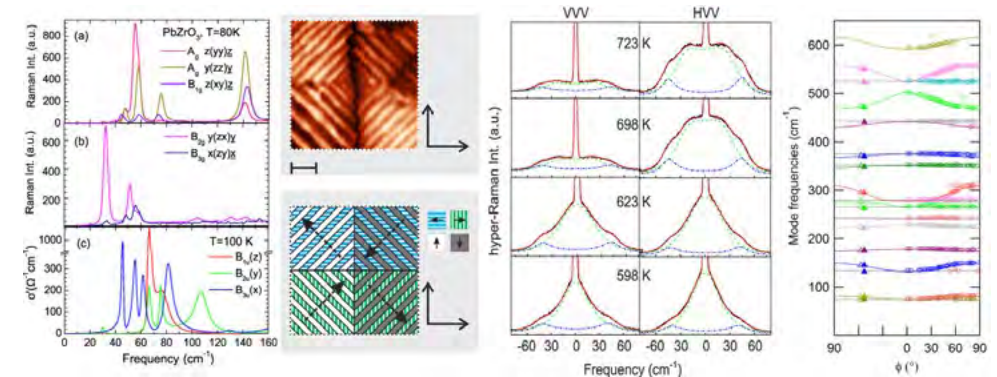


**Fig. 5:** Liquid crystalline textures observed under polarizing microscope in a blue phase (BP) and at the cholesteric-TGBC phase transition. Widths of figures correspond to 100  $\mu\text{m}$ .

Another topic of practical interest concerns macroscopic properties of mixtures composed of liquid crystalline compounds with fundamentally different properties. Innovative discovery has been made by blending achiral hockey-stick molecules with a chiral rod-like liquid crystalline compound. By tailoring the composition, several frustrated phases (blue phases, twist-grain-boundary (TGB) phases) have been induced in a broad temperature and concentration ranges, none of them existing in the starting compounds. The unique interaction between hockey-stick and chiral rod-like molecules was shown to be beneficial for convenient properties, e.g. for increased spontaneous ferroelectric polarization. [9].

### Spectroscopic Microscopy: Expertise in Perovskite Crystals

Leading research activities in the spectroscopic microscopy laboratory comprise investigation of lattice dynamics in inhomogeneous materials or in materials available in very small dimensions. For example, our current equipment allows the probing of THz-range polarized Raman spectra from the same few micron-sized area that has been probed in parallel by the atomic force microscope, or to follow changes in Raman spectra across the field or temperature induced phase transition. Significant effort has been paid to technical improvements of the experimental set-up facilitating, for

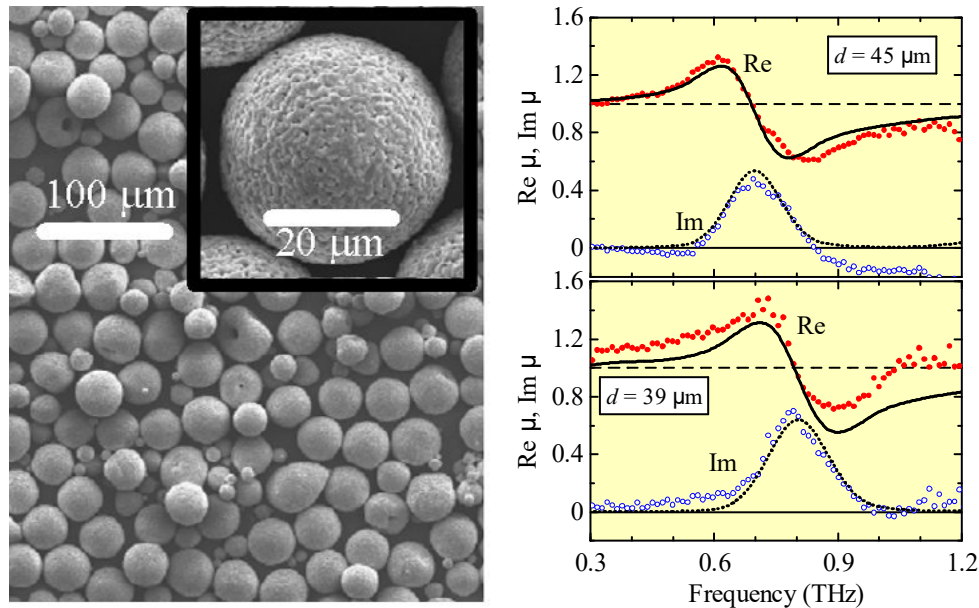


**Fig. 6:** Selected results of the Spectroscopic microscopy laboratory. From left to right: polarization analysis allows us to distinguish various soft mode crystal lattice vibrations in Raman and dielectric spectra of antiferroelectric lead zirconate; characteristic quadrant-quadruple ferroelectric domain pattern identified in a combined Raman-piezoforce scanning microscopy study of lead titanate thin films; hyper-Raman spectra of lead-based relaxor perovskite reveal an anomalous soft mode excitation; directional frequency dispersion of Raman-active modes of bismuth ferrite. The latter result was used to clarify controversy about the phonon mode assignment of this important multiferroic material.

example, automatic polarization measurement and analysis or detection of ultra-low frequency phonon modes in the sub-THz spectral range. Experienced members of our laboratory often advise external users and they also frequently participate in niche light-scattering experiments abroad. Spectroscopic microscopy techniques were particularly useful for example in our recent work, where we succeeded in identifying the mechanism of the antiferroelectric phase transition of lead-zirconate [10], or in studies revealing the influence of crystal substrate on domain patterns in ferroelectric films [11], and in studies of critical fluctuations of lead-based perovskites [12, 13]. We have also developed novel method for determining directional phonon dispersion in piezoelectric materials. This method proved to be useful for example in probing the grain orientation in coarse-grain ceramics of  $\text{BiFeO}_3$  [14].

### Metamaterials for the Terahertz Spectral Region

Among the most successful current research directions in the Terahertz (THz) Spectroscopy laboratory are studies of properties of artificial structures exhibiting tuneable photonic resonances in the THz spectral range. In particular, the team aims to design metamaterials and photonic crystals with optical properties controllable by external parameters such as electric field, illumination or temperature. In metamaterials, the structuring is made at a subwavelength scale such that the incident light cannot resolve those patterns and the optical properties of metamaterial samples can be described by effective parameters (effective permittivity and effective permeability). A proper choice of constituent materials and of their geometry can induce unusual electromagnetic behaviour of the metamaterial. In this way, it is possible to conceive, e.g., a medium



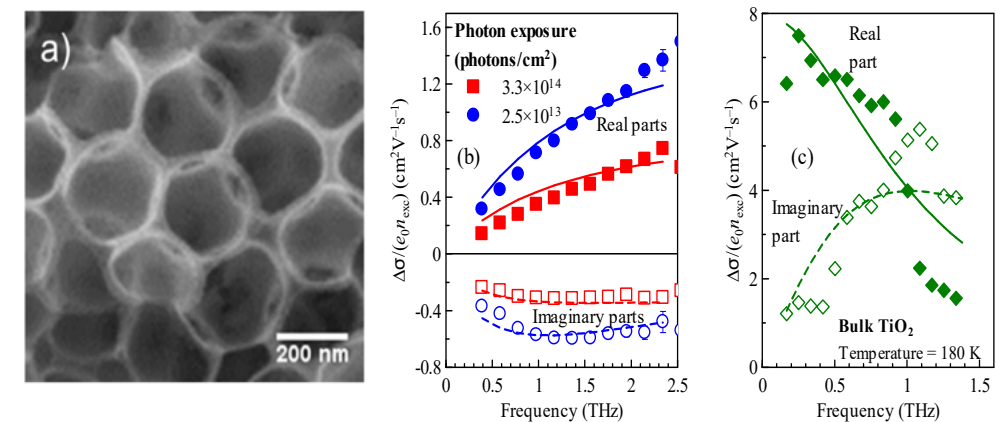
**Fig. 7:** Left: Scanning electron microscope images of the fabricated  $\text{TiO}_2$  microspheres before the sorting procedure. Sorting procedure allows one to obtain a narrower distribution of microsphere diameters  $d$ . Right: effective magnetic response (real and imaginary part of the effective permeability) of samples with a 10 % volume filling fraction of  $\text{TiO}_2$  microspheres and their sizes  $d = 45 \pm 4 \mu\text{m}$  and  $39 \pm 3 \mu\text{m}$ . Symbols: experiment, lines: results of electromagnetic simulations.

with a negative refractive index (i.e., with simultaneously negative dielectric permittivity and magnetic permeability) allowing the diffraction limit in optical imaging to be overcome. An example of such a structure is a thin layer of rutile microspheres prepared by spray-drying of a suspension of  $\text{TiO}_2$  nanoparticles which then self-assemble into microspheres. Indeed, although the crystals of rutile ( $\text{TiO}_2$ ) do not exhibit magnetic properties, the team has experimentally demonstrated that the proposed layer shows a magnetic resonance close to 1 THz with a possibility to achieve a negative effective magnetic permeability. The team has also developed methods of unambiguous simultaneous determination of dielectric and magnetic response of metamaterials [15].

### Charge Carrier Transport on Nanoscale Studied by Terahertz Spectroscopy

Charge transport in semiconductor nanostructures is a key process in a number of applications, including photovoltaic devices such as Grätzel cells. Investigation using classical (electrical) methods is limited by the requirement of electrodes attached to nanometer-sized objects. In such a situation, it is possible to take advantage of the terahertz time-resolved spectroscopy which enables non-contact measurement of nanoscale charge carrier transport with picosecond time resolution.

We have developed theoretical approaches which directly relate the measured terahertz response with charge transport processes described on the microscopic level, and which are applicable to disordered materials used in real devices. These include two key steps [16]: (1) description of the microscopic terahertz response of nano-objects which we usually calculate by Monte-Carlo simulations [17] and (2) evaluation of the role of depolarization fields which inherently develop in inhomogeneous samples for which we have developed a suitable effective medium theory approach: [18–20]. Application of these ideas allowed us to discover, e.g., electron–cation interaction in dye-sensitized  $\text{ZnO}$  nanoparticles [21] and very efficient inter-particle charge transport in  $\text{CdS}$  films prepared by chemical bath deposition [22].



**Fig. 8:** (a) Scanning electron microscopy image (top view) of calcined macroporous titania ( $\text{TiO}_2$ ) films obtained by a co-assembly of poly(methyl methacrylate) beads and sol-gel derived titania, another (b) spectrum of transient conductivity  $\Delta\sigma$  normalized by photoexcited charge density  $e_0 n_{\text{exc}}$ . No signature of Drude response is observed and  $\Delta\sigma/e_0 n_{\text{exc}}$  strongly depends on the pump photon exposure: it points out the crucial role of the depolarization fields in the structure. (c) For comparison we show the spectrum of normalized transient conductivity of bulk  $\text{TiO}_2$  exhibiting the standard Drude response.



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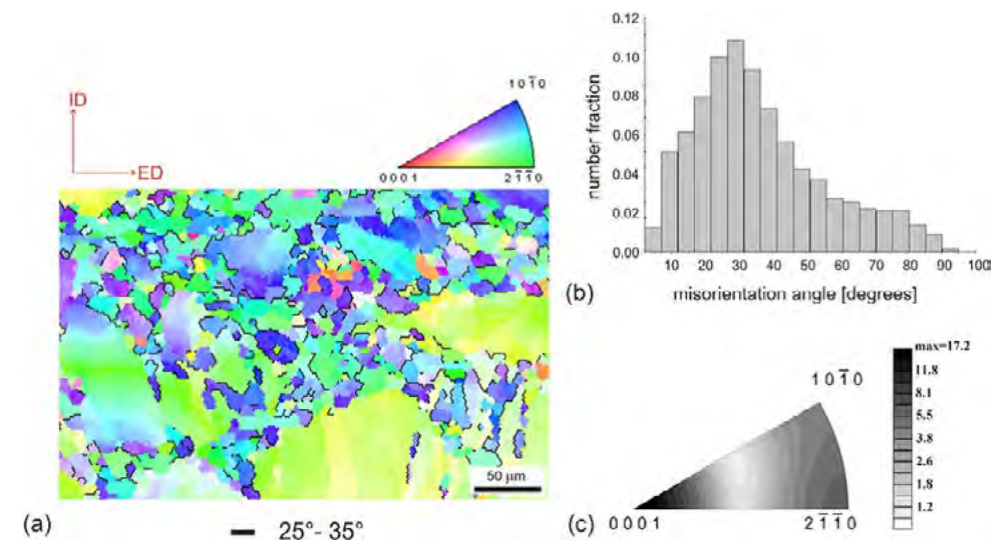
## Department of Advanced Structural Materials

Research activities are primarily focused on the preparation and characterization of physical and chemical properties of ultra-fine grained and nanocrystalline metal-based materials. These studies use the long-term experience of the staff in studies of extended defects in solids such as dislocations and grain boundaries. The department is divided into two parts, the research group “Nanostructured Materials and Interfaces” and the operating X-ray laboratory “ROTAN”. The latter laboratory is equipped with powerful sources of X-rays with a rotating anode Rigaku RU 300, a powder X-ray diffractometer PANalytical X’pert PRO and standard X-ray sources complemented by the necessary detectors. The ROTAN laboratory has been established to provide instrumental capacities and measurement time for internal and external researchers. The former group mainly conducts specific research in the fields of severe plastic deformation, nanomechanical properties, hydrogen storage, and biodegradable and biocompatible materials. Due to possession of a set of high performance electron microscopes combined with long-term experience in operation, the group is also a part of the Laboratory for Nanostructures and Nanomaterials included in the Roadmap of the Czech Research Infrastructures.

### Research Highlights

#### 30° Peak on the Misorientation Angle Distribution

It is well known that severe plastic deformation changes not only grain size but also other microstructural parameters. In the case of equal channel angular pressing (ECAP), the grains mutually misoriented by approximately 30° are most frequently observed in magnesium (Fig. 1). Many works reported a similar maximum in misorientation angle distribution for wrought magnesium and its alloys but the exact reason for its occurrence was unclear. Their authors usually speculated that this could be caused by double twinning. The comparison of the microstructure of magnesium deformed by ECAP at 234 °C with theoretical calculations enabled us to explain the high frequency of this orientation relationship: We showed that this is the consequence of the preferential occurrence of special grain boundaries. Obviously, the grain boundaries with these orientation relationships possess lower energy than other grain boundaries and therefore, their formation is energetically more advantageous [1].



**Fig. 1:** Grain orientations in ECAPed magnesium. (a) The grain boundaries misoriented by  $30^\circ \pm 5^\circ$  are marked in black; (b) histogram of the frequency of the misorientation angle; (c) distribution of the rotation axes for the  $30^\circ \pm 5^\circ$  misorientation relationship.

### Room-Temperature Double-Twinning

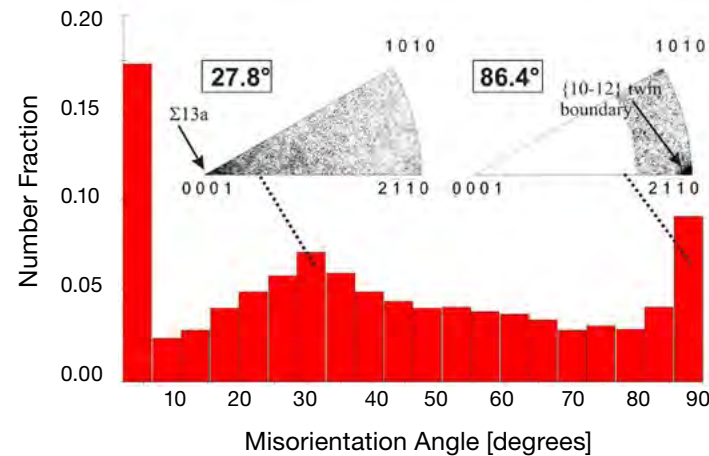
Deformation twinning is an important mechanism of plastic deformation in hexagonal metals which maintain their original crystallography but change their orientation. The twinning can also occur inside another twin and this process is called double twinning. It has been supposed that double twinning can only occur on  $\{10\bar{1}1\}$ – $\{10\bar{1}2\}$  and  $\{10\bar{1}3\}$ – $\{10\bar{1}2\}$  crystallographic planes. However, in 2011 the first publication on twinning at the  $\{10\bar{1}2\}$ – $\{10\bar{1}2\}$  planes appeared in which these twins were observed only at low temperatures (–200 °C). Our experiments on the Mg–0.3at.% Al alloy and on Mg single crystals submitted to severe plastic deformation showed for the first time that  $\{10\bar{1}2\}$ – $\{10\bar{1}2\}$  double twinning occurs not only at low temperatures but also at room temperature and even at +160 °C [2].

### ECAP of Magnesium Single Crystals

Although hexagonal metals such as magnesium belong to the group of difficult-to-work materials due to an insufficient number of active slip systems operating at room temperature, we showed that polycrystalline magnesium can be successfully processed via ECAP at room temperature by different routes (different rotations between successive passes) provided a back-pressure is used. An investigation of the microstructure and texture by electron back-scattering (EBSD) technique consequently revealed that magnesium fully recrystallizes even at room temperature



and forms most frequently either  $\{10\bar{1}2\}$  twin boundaries or low- $\Sigma$  ones [3]. This can be seen in Fig. 2. To explain the mechanism of formation of new grains during such a complex process, we investigated ECAP of Mg single crystals. In this case we applied only a single pass of ECAP at a temperature of 230 °C without back-pressure. For interpretation of the results we modified the visco-plastic self-consistent model which enabled us to reproduce the texture, grain rotation and distribution of CSL grain boundaries. The model is based on possible dislocation reactions in different slip systems. A comparison of the modeling with EBSD data for various orientations of single crystals showed that our model offers much better results than other existing models and also enabled us to predict the distribution of various types of grain boundaries [4].

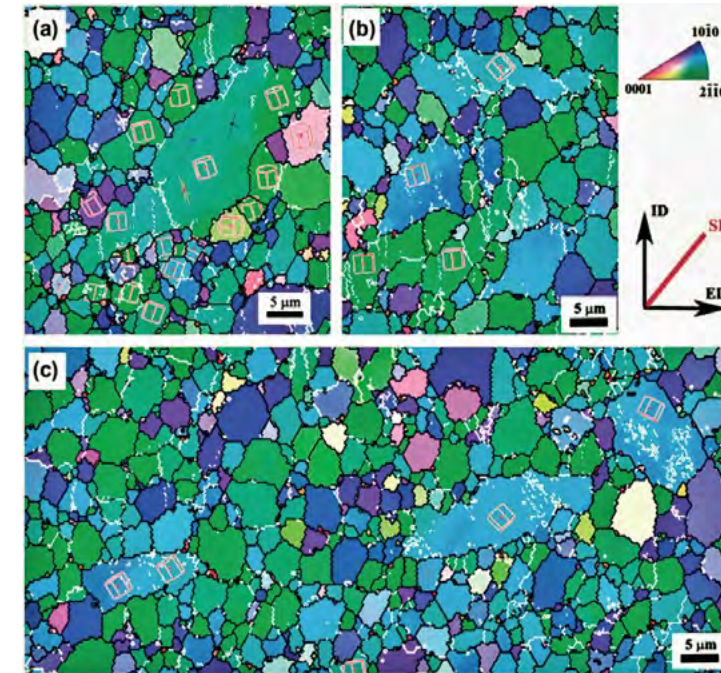


**Fig. 2:** Distribution of misorientation angles ( $>2^\circ$ ) for magnesium after 4 times ECAP processing with back-pressure at RT. The two peaks correspond to the misorientations  $27.8^\circ$  ( $\Sigma 13$  CSL grain boundary  $\{10\bar{1}2\}$ ) and  $86.4^\circ$  (twin boundaries).

### Structure/Property Relationship in ECAPed AZ31 Alloy

The study of the structure of the Mg–3wt.% Al–1wt.% Zn (AZ31) alloy during passes via ECAP with gradually decreasing temperature showed that the lowest temperature for crack-free processing is  $\sim 150$  °C. It was found that distribution of the grain boundaries is qualitatively the same for all consecutive steps of ECAP: the (0001) and  $\{11\bar{2}2\}$  planes in large (unrecrystallized) grains were parallel to the slip plane (Fig. 3). Measurements of the tensile deformation confirmed that mechanical properties of ultrafine-grained AZ31 alloy after ECAP at different consecutive temperatures are affected by final texture and twinning [5]. Based on the obtained results we improved the prediction capability of the conventional visco-plastic mod-

el [6]. We also found that the effect of slip deformation on formation of the texture in AZ31 alloy cannot be neglected even in the cases where atomic mixing (shuffling) is more significant than slip. The existence of the  $\{10\bar{1}2\}$  twin boundary can thus be expected in any case supposing the compatibility conditions are fulfilled. Possible deviations are only caused by dislocations [7].

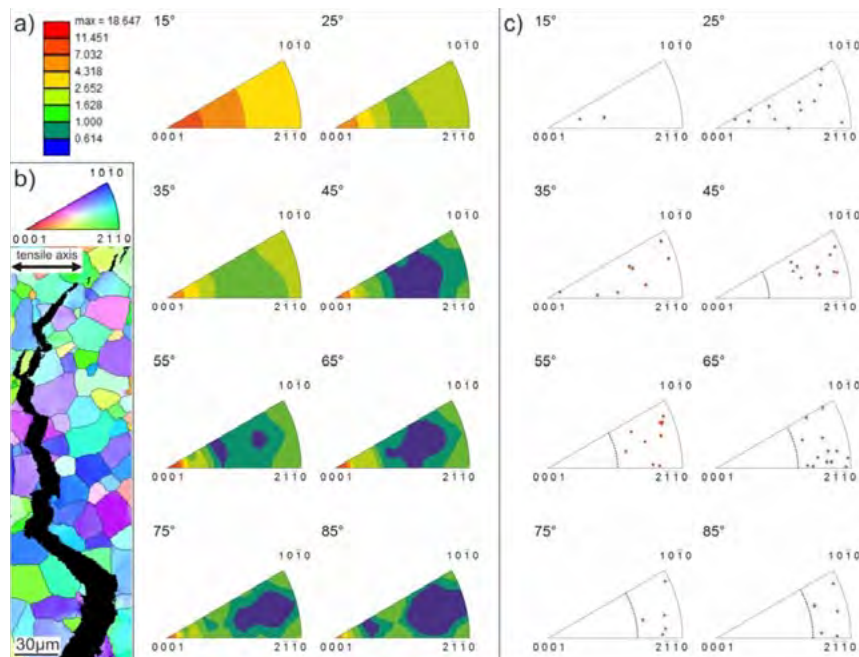


**Fig. 3:** Large prolonged grains appeared after ECAP decrease with the consecutively decreased pass temperature,  $2 \times 250$  °C +  $2 \times 200$  °C. Colours of the planes of the prolonged grains: (0001) – blue,  $\{10\bar{1}0\}$  – red,  $\{11\bar{2}2\}$  – black. The directions of the reference axes with the slip plane normal are also marked.

### Fracture of Titanium

Crack development plays a crucial role in all materials submitted to mechanical loading. Pure titanium with a duplex microstructure was used as a model material to characterize the fracture mechanisms that occurred during quasi-static tensile loading at room temperature [8]. The duplex microstructure was composed of  $\alpha$  grains decorated by a small fraction of  $\beta$  phase along the grain boundaries and at triple junctions thus resembling the microstructure of many commercial Ti alloys. It has been found that the fracture mechanism involves both transgranular and intergranular cracking. Transgranular cracking is a much more common

fracture mechanism. By comparing EBSD data with simulations, it was possible to denote the most probable crystallographic planes in grains with a hexagonal, close packed structure susceptible to transgranular cracking. Intergranular failure unambiguously prefers general grain boundaries, and all special boundaries are more resistant (Fig. 4).



**Fig. 4:** (a) Misorientation distribution function (MDF) of grain boundaries for a crack-free microstructure; (b) typical EBSD map in ED-TD plane oriented with respect to the tensile direction for one of the investigated cracks; (c) discrete misorientation values for intergranular cracking between formerly neighboring grains.

### Grain Boundary Segregation

One of the important results, reflecting the long-term effort in studies of grain boundary properties in this Department, is the book of P. Lejček, “Grain Boundary Segregation in Metals” [9]. As is apparent from the above discussion, grain boundaries are important structural components of nano- and polycrystalline materials used in the vast majority of technical applications. Because the grain boundaries form a continuous network throughout the materials, their properties strongly affect the materials’ practical use. One of the phenomena which seriously affect the application of materials is solute segregation at grain boundaries. On one hand, it re-

sults in the loss of grain boundary cohesion and consequently, in brittle fracture of the polycrystalline material, on the other hand it plays an important role in grain size stabilization and preservation of nanocrystalline materials at higher temperatures. The book *Grain Boundary Segregation in Metals* deals with the fundamentals of grain boundary segregation in metallic materials such as description of the structure and thermodynamics of grain boundaries, approaches to the study of grain boundary segregation, and models of equilibrium segregation and its relationship to grain boundary structure, classification, grain size, pressure, and other material properties (grain boundary cohesion, corrosion and diffusion) including the fundamentals of the grain boundary engineering concept. It serves both for the specialist in the field (as documented by the already large number of citations) as well as those studying material for master and doctoral theses.



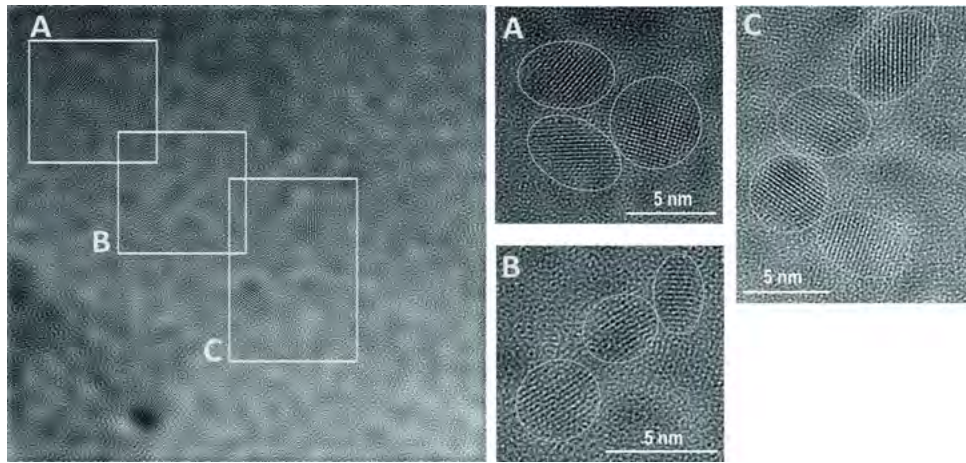
**Fig. 5:** The book *Grain Boundary Segregation in Metals* written by P. Lejček.

### MgO nanoparticles

In the field of green chemistry, we succeeded in the synthesis of nanoscale MgO particles by a new route using catalyzed corrosion with the sol-gel method at room temperature with subsequent annealing [10]. Instead of the usually used halogens to accelerate the reaction, the starting material was Mg with a small amount of Zn in a solid solution (Mg-0.11at.% Zn) and methanol. The presence of Zn in the Mg solid solution catalyzed the reaction due to formation of micro-galvanic cells between Mg and Zn. The product of the reaction ( $\text{Mg}(\text{OCH}_3)_2$ ) was subsequently dried and annealed in air without supercritical drying to gain MgO nanoparticles. Characterization revealed a narrow size distribution of MgO nanoparticles with diame-



ter of ~5 nm and without trace of residual groups (Fig. 6). The concentration of Zn in resulting MgO powder did not exceed 100 ppm.



**Fig. 6:** High resolution transmission electron microscopy of MgO nanoparticles (white circles)

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## Department of Functional Materials

The department (<http://ofm.fzu.cz/>) was only established in January 2009 with P. Sittner as the head. It brought together two groups of mostly young researchers working actively in the field of functional engineering materials and nanostructured diamond thin films and has grown substantially to encompass four research groups in 2014. These are; Functional Materials and Composites, Materials for Nanosystems and Biointerfaces, Magnetic Shape Memory and Magnetocaloric Materials, and Physical Properties of Biomaterials. Current research activities focus on advanced functional materials exhibiting martensitic phase transformations such as ferroelastic shape memory alloys, ferromagnetic Heusler alloys, chemical vapour deposition (CVD) of nanodiamond thin film coatings and physical studies of organic systems. Though these areas seem to be rather different, there are uniting links consisting of: i) functionality imprinted at the atomic level, ii) a physical approach to solve problems and iii) medical applications. It took nearly five years to build the indispensable experimental base of the department, particularly to develop the laboratories for thermomechanical testing, CVD nanodiamond coating, smart magnetic materials, metallurgy, sample preparation, material characterization and advanced microscopy (SEM, AFM). The department's researchers have participated in more than 20 national projects and 15 European projects with large scale industrial partnerships. International PhD student training has been carried out within the framework of the national centre of excellence AdMAT, two European Marie-Curie research training networks MATCON and MULTIMAT, the FZU-ESRF PhD project and the French undergraduate student training program. The department organized two major international conferences focusing on martensitic transformations in Prague – ESOMAT 2009 and SMST 2013. The researchers collaborate within a Czech–German consortium involved in the design and construction of the Beamline for European Material Engineering Research (BEER) to be built at European Spallation Source in Lund, Sweden by 2020.

### Research Highlights

#### Functional Materials and Composites

The research of the group deals with unique functions exhibited by materials undergoing martensitic phase transformation, especially ferroelastic shape memory alloys. The diffusionless martensitic transformation taking place upon cooling and/or loading introduces a vast number of internal interfaces into the product's martensite phase. These interfaces are highly mobile and can be manipulated by external fields – stress, temperature, magnetic field. Since the motion of interfaces results in reversible changes of macroscopic shape, this gives rise to unique thermo-magneto-mechanical functional responses frequently utilized in innovative engineering applica-

tions such as simple and reliable actuators, motors, vibration dampers, etc., scalable down to the submicron range.

Figure 1 provides an overview of the group's research. The team lead by L. Heller has developed a wide range of new thermomechanical testing methods for the application of static and dynamic loads to thin metallic filaments. A variety of unique instruments was designed and built for application of these methods both in the home laboratory and externally at large scale facilities, e.g. ESRF [1]. A set of experimental data obtained on ultrathin NiTi filaments tested for combined tension and torsion over a wide temperature range using this equipment was provided free on the internet [2] and used by researchers worldwide to benchmark constitutive models of NiTi. The researchers have developed [3] and patented [4] an **electropulse heat treatment method to set the shape and manipulate microstructures and functional properties of continuous NiTi filaments** over a millisecond time range. Combined with time resolved synchrotron X-ray diffraction, the electropulse method

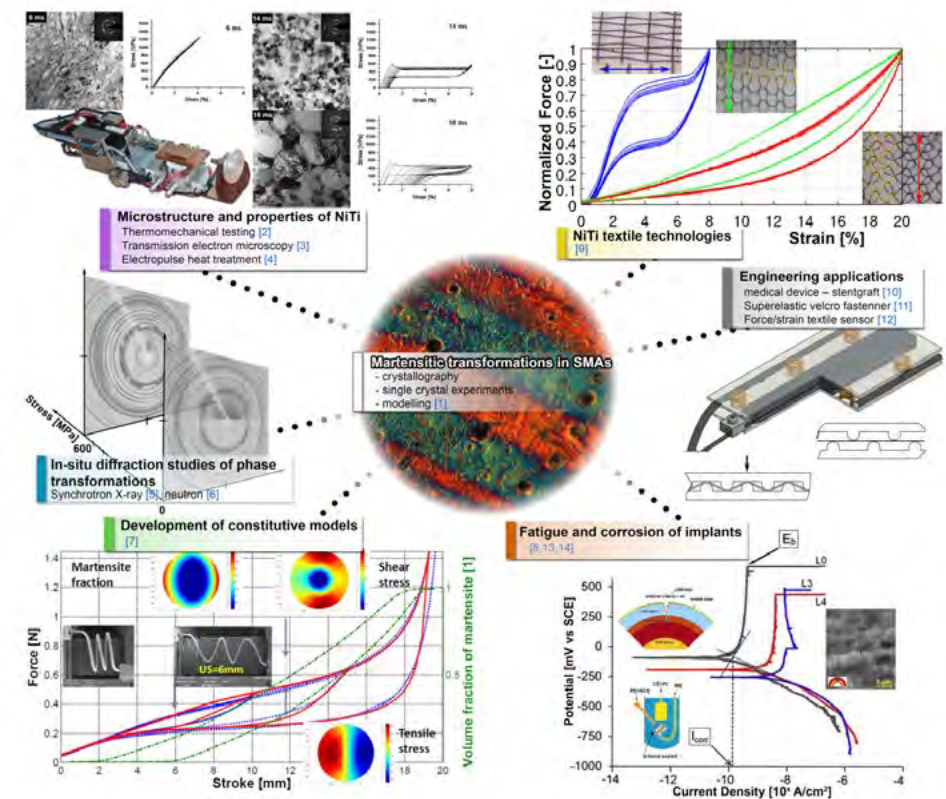


Fig. 1: Current NiTi technology research in the department



enabled us to investigate the extremely fast processes taking place in thermomechanically treated metallic filaments undergoing dynamic recovery and recrystallization [5]. Further novel experimental methods, such as 3D X-ray diffraction, were recently applied to investigate *grain resolved internal stress and buried interfaces* propagating during localized deformation of tensioned NiTi wire. Internal stresses generated by NiTi inserts embedded in steel plates during heating were evaluated by neutron strain scanning combined with FE simulation [6]. The researchers developed constitutive models for NiTi shape memory alloys [7] and applied them to simulate thermomechanical behaviours of various complex NiTi elements as superelastic springs [8] or shape memory textiles [9].

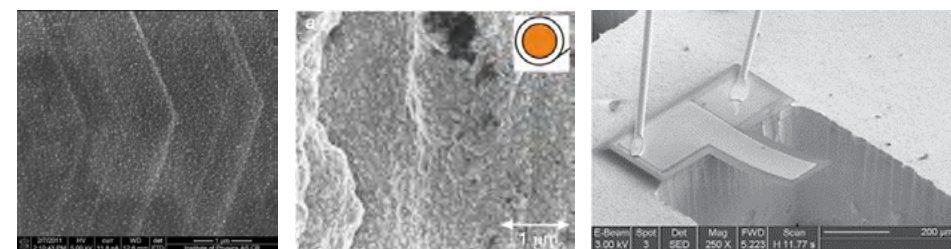
The main recent achievements group are in the design and development of hybrid functional textiles with NiTi filaments [9]. This work has been carried out since 2004, in collaboration with industrial and academic partners providing indispensable textile expertise. These functional textiles inherit their unique properties from the NiTi filaments and transform them to the 2D form, which opens the way for the development of **shape memory textile technologies**. Several patents were filed, e.g. the Medical Device – Stentgraft [10], Velcro-like fastener with superelastic NiTi hooks [11] or innovative force/strain sensor for application within textile structures [12].

Finally, preliminary fatigue failures of braided esophageal NiTi stents in aggressive biofluids deforming periodically when implanted into the human body were investigated (in collaboration with stent producer Ella-CS). The braided NiTi stent was substituted by a helical NiTi spring, manufactured by the same technological route. This was subjected to cyclic mechanical loads in corrosive fluids and its corrosion fatigue performance was evaluated [13]. Novel in-situ electrochemical methods [14] were developed to monitor the accumulation of mechanochemical damage during the cyclic tensile tests on NiTi wires and springs. The **origin of the random preliminary failure of NiTi stents** deforming in fluids was rationalized by the newly proposed fatigue degradation mechanism [14] involving mechanochemical damage to the TiO<sub>2</sub> surface oxide, hydrogen accumulation, transport, local suppression of the martensitic transformation and consequent NiTi embrittlement.

### Materials for Nanosystems and Biointerfaces

The group was set up in 2009 by M. Nesládek, a world recognized expert in nanodiamond thin film technologies, who returned to the institute after a 20 year research career in Belgium and France. Together with F. Fendrych, he built a unique laboratory for preparation of the chemical vapour deposition (CVD) of nanodiamond film coatings over large areas, on 3D surfaces and at low temperatures [15]. Diamond films, in their various crystalline forms, have many potential industrial applications in the fields of mechanical and chemical protective coatings, biocompatible coatings, optics, electronics and electrochemistry. Electrical properties of nanodiamond films for biosensor or photovoltaic applications were adjusted by Boron doping [16, 17], nanocrystalline coated silicon solar cells were prepared for direct photoelectro-

chemical water splitting [18]. In the medical field, a nanocrystalline diamond coated stainless steel coronary stent showed promising results after the implantation into pig arteries [19] and nanocrystalline diamond particles have been investigated for their use in drug delivery systems [20]. Several interesting applications of nanodiamond coatings in the medical field, energy conversion and sensor areas were developed in collaboration within the large scale national nanotechnology project BLOKOM coordinated by M. Nesládek.



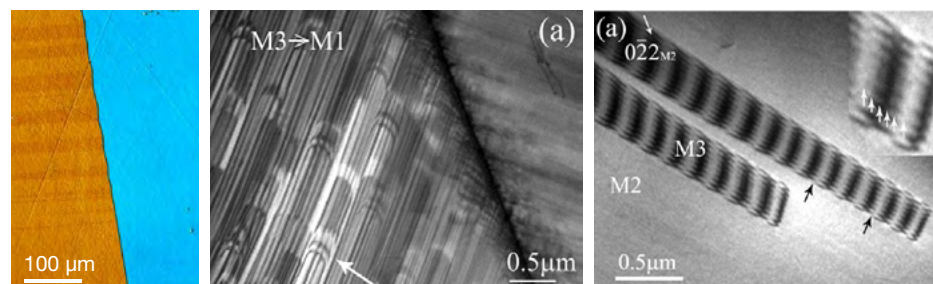
**Fig. 2:** Nanodiamond coatings on coronary stents for enhanced biocompatibility (left), Zr rod for nuclear fuel cladding (middle) and diamond/AlN micro-cantilever for MEMS sensor (right).

After M. Nesládek left the department his position was taken by V. Mortet, a senior researcher from LAAS-CNRS in Toulouse, France, who joined the department in 2013 as a Purkyně fellow. He took over the leadership of the group and also brought in new research of (bio-)micro-electro-mechanical systems and acoustic bio-sensors which require sophisticated patterning of diamond films and multilayers by laser lithography. The researchers lead by I. Kratochvílová have recently succeeded in coating zirconium alloy rods used as a nuclear fuel cladding by polycrystalline diamond layers using the microwave plasma enhanced chemical vapour deposition method [21]. This **diamond coating protects the zirconium alloy cladding against undesirable oxidation** under severe vapour pressure and high temperature conditions occurring in nuclear reactors. The technology was patented and further research is in progress.

### Magnetic Shape Memory and Magnetocaloric Materials

The research interests of the group focus mainly on multiferroic materials, mostly Heusler alloys, which exhibit new kinds of functional behaviour involving magnetism. The group is led by O. Heczko, a world recognized expert on magnetic shape memory, who joined the department in 2009 as a Purkyně Fellow after 10 years working in Finland and Germany. The ferromagnetic shape memory materials exhibit large strains of several percent in response to the variation of a relatively weak external magnetic field. The effect is conditioned by the coupling of strong magnetic anisotropy with high mobility of twin boundaries in these materials. Heczko and his colleagues proposed a new interpretation of the so called modulated martensite as an

adaptive phase which may explain high mobility of twin boundaries in general [22]. More recently the group's researchers have discovered a new type of extremely highly mobile twin boundary [23] and explained the very complex interfacial microstructure behind it [24]. An example of a single highly mobile macrotwin boundary with modulation twinning is visible in the figure 3. The mobility of this kind of boundary is nearly independent of temperature thus the magnetic shape memory effect can exist at very low temperatures down to a few Kelvins [25]. This motivated the group to start new a research program focusing on evolution of elastic properties during the martensitic transformation [27]. The elasticity of the cubic parent phase (austenite) was expected to be simple but surprisingly the experimental results indicate quite complex behaviour [26]. **A complementary in-situ transmission electron microscope study [28] revealed the mechanism of twin boundary motion** in non-modulated martensite at the atomic microscopic scale. The Figure 3 is a snapshot of the twinning process in the martensite phase by the motion of twinning dislocations in the twinning planes (middle) and their detailed ex-situ analysis (right). As well as the Ni–Mn–Ga research, the group also studies other ferromagnetic shape memory alloys such as Co–Ni–Al and their magneto-elastic properties [29].



**Fig. 3:** Mobile twin interfaces in NiMnGa magnetic shape memory alloy martensite.

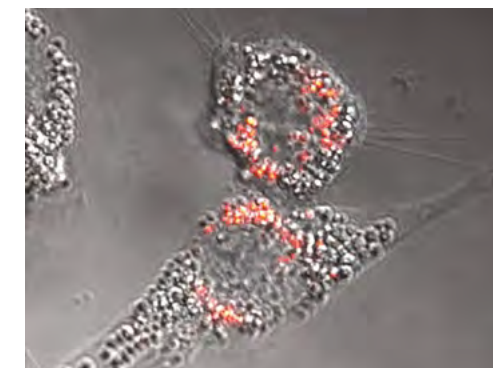
The group grew significantly in 2013 when I. Tomáš, M. Jirsa and other colleagues joined the department. I. Tomáš has been working for long time on **the development of a non-destructive magnetic method for the evaluation of fatigue damage of ferromagnetic engineering materials**. The in-situ method they developed and patented [30] uses the evaluation of magnetization processes reflecting gradual changes of microstructure during the lifetime of the engineering component. Recently, this was successfully applied to test degradation of nuclear reactor steel due to neutron radiation [31] and to evaluate high-cycle fatigue damage of industrial construction steel [32].

Under the leadership of J. Kopeček, the group has built a metallurgy laboratory with alloy casting, single crystal growth, heat treatment, and metallography facilities. Recently, they installed a new scanning electron microscope with focused ion beam. This modern SEM-FIB facility has become a core of the newly built interdisciplinary

centre SAFMAT. These facilities will also be used by PhD students trained within the Centre of Excellence AdMAT focussing on advanced engineering materials research.

### Physical Properties of Biomaterials

The research group under the leadership of I. Kratochvílová was set up in 2014 by the department's researchers involved in biophysics research. Research dealing with functionalized nanodiamond particles for application in optically-traceable intracellular nanodiamond sensors was the topic of the Ph.D. thesis of two excellent students V. Petráková and A. Kovalenko who left the department in 2013. They have proven the applicability of nanodiamonds as cell markers traceable by their luminescence in the confocal microscope (Fig. 4). The results were published in high impact scientific journals [20, 33] and attracted significant attention not only within the scientific community but also in the general media. The group has collaborated with other academic and industrial teams focusing on the development of recombinant vaccines and biocompatible drug carriers.



**Fig. 4:** Confocal microscope picture of IC21 cells marked by fluorescent nanodiamond particles.

Group members modelled the stability of the construction of the vaccine against Lyme borreliosis and analyzed the influence of selected parameters on individual parts of the complex. Based on their results key parts of the vaccine were constructed [34]. Mutual cooperation between academia and industry allowed application of this technology to prepare antigens, adjuvants synthesis, liposomal carriers, and to carry out vaccine design and tests. Preclinical experiments demonstrated the ability of the vaccine to induce a significant antibody response. The research was successfully completed by carrying out PCT searches and filing national patent applications [35]. Discovery of the new vaccine against Lyme borreliosis was widely reported in the media. For this research I. Kratochvílová obtained two awards, Co-operation of the Year 2014 and the award of the Technology Agency of the Czech Republic, and was even nominated for the prestigious national award Česká hlava 2014.

Together with the Faculty of Medicine of the Charles University, University of Wyoming, USA and the centers of reproduction medicine (ISCARE, Genetics and reproduction medicine center GENNET), the team currently investigates the influence of cultivation and the method of achieving extremely low temperatures on cell condition. Current activities of the group also represent a key part of the biophysics



research within the interdisciplinary centre FUNBIO-SAFMAT, particularly the development of atomic force microscopy facilities for organic materials, characterization of functionalized thin films and in-vivo imaging of living cells.

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## Department of Condensed Matter Theory

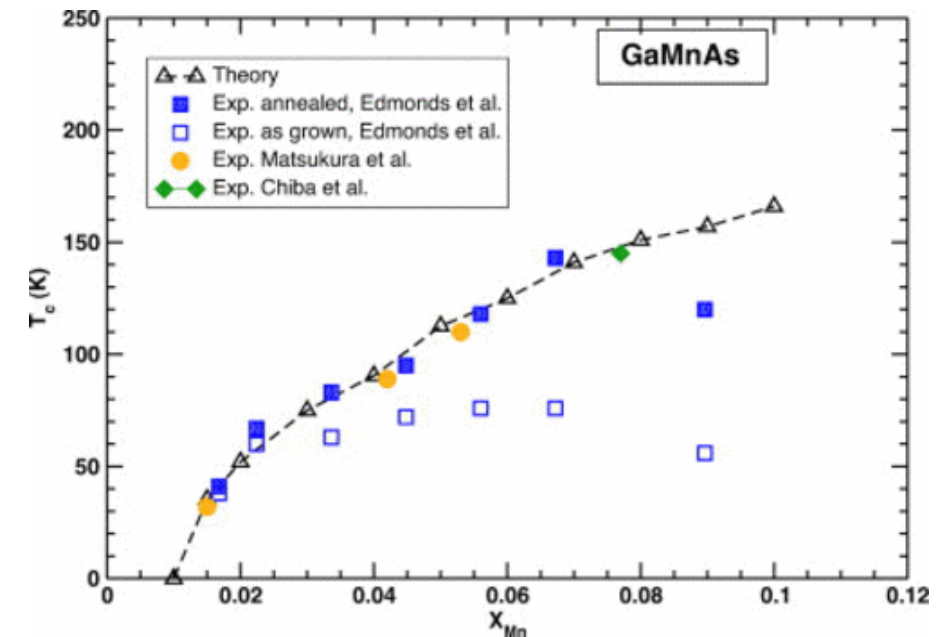
The research in the department covers description of the electronic, magnetic and transport properties of solids, in particular of systems with a nontrivial complex structure of the elementary cell, broken or reduced translational symmetry or of systems in extreme conditions in and out of thermodynamic equilibrium on microscopic, nanoscopic and macroscopic scales. We use and develop for this purpose advanced techniques of equilibrium and non-equilibrium classical and quantum statistical mechanics, many-body Green's functions, large-scale first-principles calculations and numerical simulations. We aim at qualitative understanding of electronic phenomena in solids on a model level as well as at a realistic quantitative description of the electronic structure of real materials.

The department consists of two partly overlapping groups of researchers. The focus of the first group has traditionally been quantum theory of electrons in metals, semiconductors and their alloys, including surfaces, interfaces, and multilayers. Recently, their research interests extended to cover nano and mesoscopic objects with more emphasis on strong electron interactions and correlation-induced quantum collective phenomena. The second research group attempts to understand macroscopic phenomena in solids in and out of thermodynamic equilibrium via microscopic modeling and numerical simulations. Disordered and frustrated complex systems are primarily of interest, for which nonstandard methods of description have to be used and developed. The outreach of these methods goes beyond the models of statistical physics to comprise informatics, networking, economics, sociology, and biology.

### Research Highlights

#### First-principles Calculations of the Electronic Structure of Semiconductors and Metals

The potential to utilize spin of the electron as a gear in electronic devices boosted research interest in magnetic impurities diluted in semiconducting materials. Our research on magnetic semiconductors was amplified in recent years by a number of international collaborations and a co-operation with the Department of Spintronics and Nanoelectronics of the Institute of Physics. Our contribution to this research direction has been in proposing empirical tight-binding models and performing large-scale ab-initio calculations of the electronic structure and magnetic and transport properties of diluted magnetic semiconductors. We showed that magnetic percolation and the atomic structure are decisive for the determination of the values of effective magnetic exchange interactions and the Curie temperature of the transition to a ferromagnetically



**Fig. 1:** Curie temperature in  $Ga_{1-x}Mn_xAs$  as a function of  $x$ . The triangles denote the calculated values within the SC-LRPA. The other symbols are the measured values for as-grown and annealed samples (from ref. [1]).

ordered state. We contributed to a review article on first-principles theory of diluted magnetic semiconductors [1] by writing the part on the calculation of the effective magnetic exchange interactions used to assess the temperature of ferromagnetic ordering.

The most technologically promising and accessible semiconductor, GaAs diluted by manganese atoms was scrutinized on both the tight-binding and ab-initio levels. Based on our calculations we explained the controversy between the experiment and the theory assuming that manganese atoms form an isolated impurity band. We showed that the impurity (Mn) band merges with the valence band of GaAs even for small concentrations of Mn atoms and the assumption of a separate impurity Mn band was false [2].

Ferromagnetic semiconductors seem not to be the only possible electronic devices with magnetic properties. Recent studies showed that semiconductors with antiferromagnetic ordering may play an even more important role in the future of spin electronics, since they are magnetic internally and not externally. We determined the electronic structure of thin films of CuMnAs by large-scale ab-initio calculations. Such films were prepared in the laboratory by epitaxial growth at room temperatures. We demonstrated that the material grown in this way is stabilized in a tetragonal structure and represents a new prospective semiconducting antiferromagnet [3]. Our ab-initio calculations also



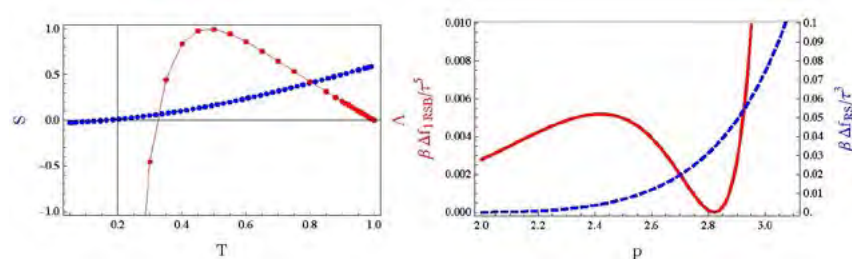
helped determine the magnetoresistance of a class of other materials from which spintronic devices with antiferromagnetic interactions could be potentially built [4, 5].

Generally, the electronic-structure community has been turning its attention to improving the density-functional theory by including neglected dynamical effects of electron correlations present in heavy metals, lanthanides and actinides. This effort combines the dynamical mean-field theory of strongly correlated materials for long length scales with quantum-mechanical first-principles computational schemes suitable for short length scales. With the synergy of this powerful multi-scale technique we quantitatively explained the position of the valence-band satellite in the ferromagnetic nickel [6] and helped elucidate the electronic structure and the role of spin fluctuations in a number of paramagnetic actinides [7, 8].

### Statistical Physics of Interacting and Frustrated Systems

Not all properties of solids can be explained from a quantum first-principles theory of the atomic and electronic structure. There are situations where long-range fluctuations or coherence blur out the details of the short-range atomic structure. Then, alternative techniques must be employed to explain and understand measurable macroscopic phenomena. Methods of thermodynamics and statistical mechanics come into play. They allow us to introduce microscopic, quantum or classical, models of co-operative phenomena observable on macroscopic length scales.

Magnetic frustration as observed in materials called spin glasses has not yet been fully understood. In particular, the question has been widely discussed as to whether a finite or infinite number of parameters determines the equilibrium glassy phase in systems without spin-reflection symmetry. We found via the asymptotic expansion below the glass ordering temperature that a solution with infinite-many and continuously distributed order parameters exists in the whole glassy phase of a mean-field Potts glass, a model with  $p > 2$  spin states without spin-reflection symmetry, even in the region where a solution with two order parameters was expected to determine



**Fig. 2:** Instability (red) and entropy (blue) as a function of temperature of the mean-field Potts glass with two order parameters (left panel) and a difference between the free energy density of the full solution with infinite number of order parameters and that with only one (blue dashed curve) or two (red solid curve) parameters as a function of the number of Potts states. Free energy is maximal in equilibrium (from ref. [9]).

the equilibrium. We showed that it is the solution with infinite-many order parameters that represents the true thermodynamic equilibrium with maximal free energy [9, 10].

A statistical macroscopic system need not consist of only microscopic atoms or molecules. Whenever a large amount of even macroscopic agents, for instance cars, animals or human beings interact and influence each other, the whole system shows universal features on large time scales that can be captured by methods of statistical mechanics. That is why modeling, that uses physical and mathematical models to simulate behavior of many interacting objects, has successfully been used in a number of non-physical and interdisciplinary fields. Modeling was in particular successful in economics and in the description of trends in the long-time behavior of financial markets. One of our recent most remarkable achievements is completion of a monograph *Essentials of Econophysics Modelling* for the prestigious publisher, the Oxford University Press. The book not only gives the best up-to-date and comprehensive overview of modeling in econophysics, it contains a number of original results achieved by the author over years [11].

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Institute of Physics  
The Czech Academy  
of Sciences

Division of Solid  
State Physics



The basic research in the division is mainly aimed at various semiconducting nanomaterials, such as silicon nanowires, InAs based quantum dots, allotropic forms of carbon, i.e. nanodiamond, and graphene, and new phosphors and materials for advanced scintillators. The Spin Hall Effect, spin-orbital and spin-light interactions are intensively studied in novel ferromagnetic and anti-ferromagnetic semiconductors. Of special interest are magnetically sensitive intermetallic alloys the phase transitions of which are systematically studied under high hydrostatic pressure. These materials were also proved to be convenient in the form of magnetic nanoparticles for medical applications. In addition, methods, such as the X-ray and electron diffraction, atomic force microscopy and low temperature magnetotransport are extensively used and continuously accommodated for the characterization of nanosystems.

The Division consists of six departments:

- Department of Semiconductors p. 111
- Department of Spintronics and Nanoelectronics p. 121
- Department of Structure Analysis p. 134
- Department of Magnetism and Superconductors p. 140
- Department of Thin Films and Nanostructures p. 148
- Department of Optical Materials p. 158

## Department of Semiconductors

### Team and Facilities

The department, having 13 scientific workers, 3 students and 8 technicians, consists of four collaborating groups, namely the: technology group (3 scientific workers), photoluminescence group (2 scientific workers), transport group (5 scientific workers) and theory group (3 scientific workers). The principal equipment of the technology group is an AIXTRON 200 MOVPE (Metal-Organic-Vapor-Phase-Epitaxy) apparatus, installed in 1994 which is still in operation (Fig. 1). During this period more than 5000 samples have been grown for basic research carried out in many institutions in the Czech Republic and abroad. The main tool of the photoluminescence group is an SDL-1 PL spectrometer with helium cryostat operating down to  $\sim 2.2$  K. The transport group has at its disposal, standard magnetotransport equipment involving a superconducting magnet (8 T), cryostats covering the temperature range 0.3–700 K, a Polaron S 4600 deep level spectrometer and an Edwards–AUTO 500 apparatus for preparation of thin films. In 2013 the groups of technology and photoluminescence were awarded by the EU Structural Fund the second prize for the project LABONIT [1], in the frame of which a new MOVPE apparatus for the preparation of nitride-based heterostructures and a Raman spectrometer for their characterization will be purchased.



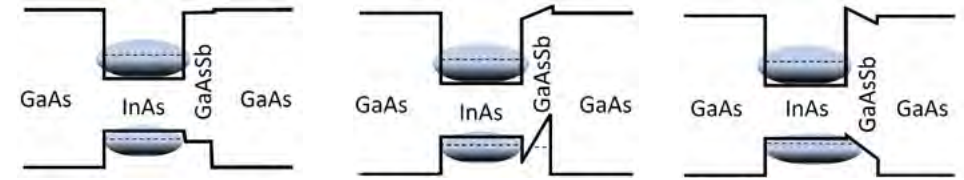
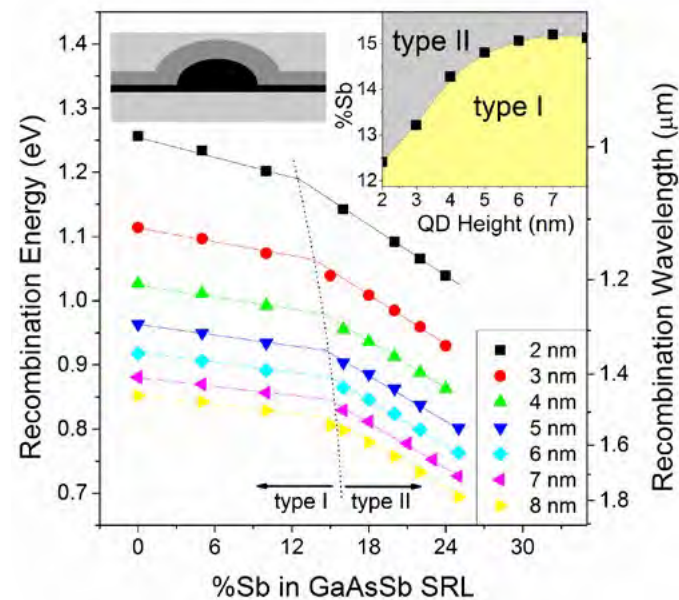
**Fig. 1:** The first commercial MOVPE apparatus AIXTRON 200 in the Czech Republic was taken over in 1994 from AEG–Ulm, Germany and installed in the Department of Semiconductors.

## Research Highlights

The principal common subjects of research of the technology and photoluminescence groups are InAs/GaAs based quantum dots prepared by MOVPE. Quantum dots (QD) are nanometric objects where the movement of electrons is confined in all three dimensions. This results in a robust discrete energy level structure which depends mainly on the size of QDs. Since the QDs imbedded in heterostructures can in principle control the optoelectronic properties of the whole system, the research in this direction is of primary importance for applications in tunable lasers, detectors, solar cells and possibly in the next generation optoelectronic devices with true quantum-mechanical functionality such as single-photon sources and quantum information processors. Reflecting these practical demands, our research was primarily oriented to a reproducible preparation of MOVPE grown heterostructures with InAs based QD emitting at the telecommunication bands of 1.3  $\mu\text{m}$  and 1.55  $\mu\text{m}$ .

In order to achieve this aim, it was necessary first to master the preparation of a self-assembled (Stranski–Krastanow) InAs QDs monolayer surrounded by GaAs layers, emitting around  $\sim 1.2 \mu\text{m}$  (e.g., [2]). For the further red shift of wavelength, various strategies were used. Required increase of the QD size was achieved mainly by capping QDs by strain reducing layers (SRLs) of InGaAs or GaAsSb, effectively preventing the dissolution of QDs. However, a GaAsSb SRL offers several advantages compared to InGaAs, particularly because it increases the PL efficiency and widens the energy gap between the ground and the first excited states. As a result, we are able at present to prepare QD structures with wavelength emission from 1.2  $\mu\text{m}$  to nearly

**Fig. 2:** Dependence of the recombination energy between ground states of electrons and holes on the composition of GaAsSb SRL for different heights of QDs. Dotted line represents the transition between type-I and type-II heterostructures. The inset shows the dependence of the type-I/type-II transition on the Sb content in the GaAsSb SRL and on the QD height [4].



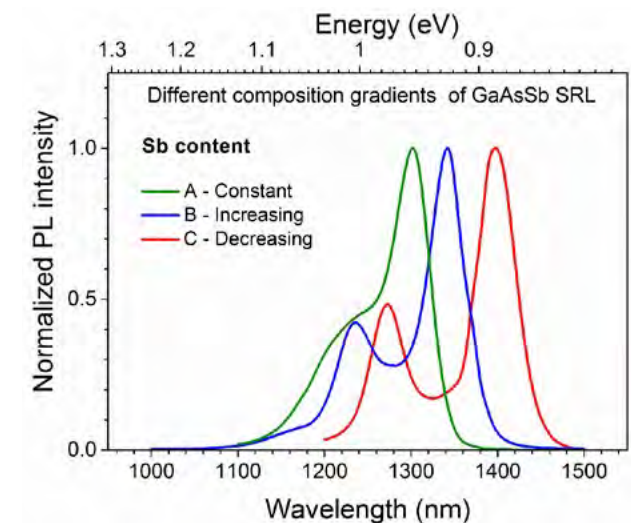
**Fig. 3:** Three types of QD structures with different Sb gradients: a) constant, b) increasing and c) decreasing.

1.8  $\mu\text{m}$  [3], this is to our knowledge the longest emitted wavelength ever reached with a InAs/GaAs QD structure.

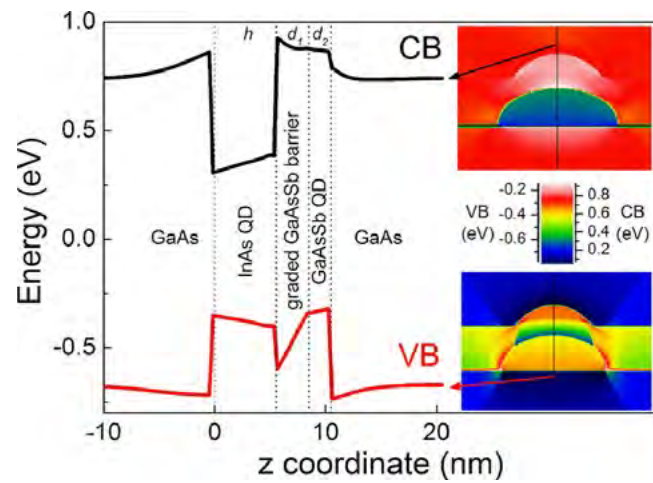
The use of GaAsSb SRL provided us also with a new tool for QD band structure engineering, enabling one to control type-I or type-II band alignment by GaAsSb composition and QD size. (Recall, in type-I electrons and holes are localized in QDs contrary to type-II, where electrons are localized in QDs and holes in SRLs.) For example, the heterostructures operating at relatively long wavelengths can also be grown intensively with more efficient photoluminescence type I band alignment. Such a possibility is due to the behavior illustrated in Fig. 2. Accordingly, the transition energy (or recombination wavelength) between the electron and hole ground states and the type of band alignment are sensitively dependent on both, Sb content and QD height, in other words, on technologically controllable parameters.

As was shown later, the band alignment is influenced not only by absolute Sb content but also by its profile [5]. The examples of three types of QD structures with different Sb profiles are shown in Fig. 3. Obviously, the most convenient profile for the wavelength prolongation is thus that with decreasing content of Sb, see Fig. 4.

**Fig. 4:** Normalized room temperature photoluminescence spectra of QD structures with 5 nm GaAsSb SRL for all three types of composition gradient – constant, decreasing and increasing.







**Fig. 5:** Calculated band alignment in the axis of vertically correlated combined InAs and  $\text{GaAs}_{0.76}\text{Sb}_{0.24}$  QDs, separated by a triangular GaAsSb barrier with graded Sb content from 10 % to 24 %. The insets demonstrate maps of the calculated valence (left scale) and conduction (right scale) band edge energies for InAs and  $\text{GaAs}_{0.76}\text{Sb}_{0.24}$  QDs in (100) cross section, the corresponding values of band edge energies along QD axis are plotted in the graph on the left.

Tailoring of the Sb profile affords another prospective application, a formation of vertically correlated combined InAs and GaAsSb QDs separated by a GaAsSb triangular barrier with increasing Sb concentration in the valence band (Fig. 5). The triangular GaAsSb barrier in the valence band separating the hole quantum states in InAs and in GaAsSb QDs, enabled us, to change their mutual energy position and band alignment separately by tuning the structure parameters [6].

Reliable knowledge of their physico-chemical parameters is necessary for successful application of metal-organic precursors to MOVPE technology. Therefore we started, in collaboration with the Institute of Chemical Technology – Prague, systematic research into vapor pressures of these toxic substances. The results of our research were highly appreciated not only by the scientific community (cf. Fig. 6, [7]) but also by renowned producers (e.g., EPICHEM, UK).

An important part of the experimental work performed in the transport group consists of the systematic measurement of the transport coefficients and deep levels in semiconductor structures, serving both as feedback information for various technological groups [8] and as a source of reliable data used for the development of models of deep impurities [9] and interfaces [10]. In addition, magnetotransport techniques were exploited in the stand-alone research into the influence of granularity on the transport properties of nanocrystalline diamond [11]. Nevertheless, attempts to characterize some new materials and structures by standard transport and impedance



**Fig. 6:** Prototype of a STAT 7 apparatus for the exact measurement of vapor pressures of metal-organic precursors developed in the frame of cooperation between the Institute and the Institute of Chemical Technology, Prague. Similar version of this model was also installed in 2011 in the NIST (formerly Bureau of Standards, USA) as an étalon apparatus.

methods revealed that substantially new approaches are necessary especially in the cases of materials with extremely high resistivity or samples with unusual topologies. This has simulated another, and possibly the most interesting activity of the transport group, work devoted to the development of original techniques and methods for investigation of semiconductor structures and, in cooperation with theoreticians, studies of the fundamental problems of measurement.

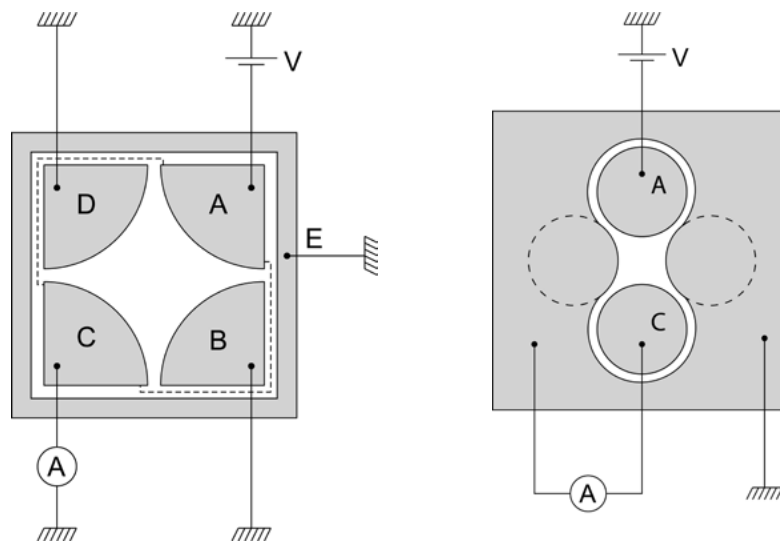
### Collaboration

In the frame of the contract US MDA-HQ0147-09-C-0005 with Kyma Technologies Inc. (NC-USA) an astonishingly simple but very effective technique was developed for the characterization of semi-insulating GaN:Fe [12]. This promising substrate material for microwave devices and optoelectronics, having an extremely small intrinsic charge concentration and conductivity  $<10^{-11}$  S/m, cannot be, unfortunately, reliably characterized by standard magnetotransport methods. Enhancement of charge carrier concentration to the measurable level was achieved by means of charge injection from a tungsten point pressed against a GaN:Fe single crystal (see Fig. 7).

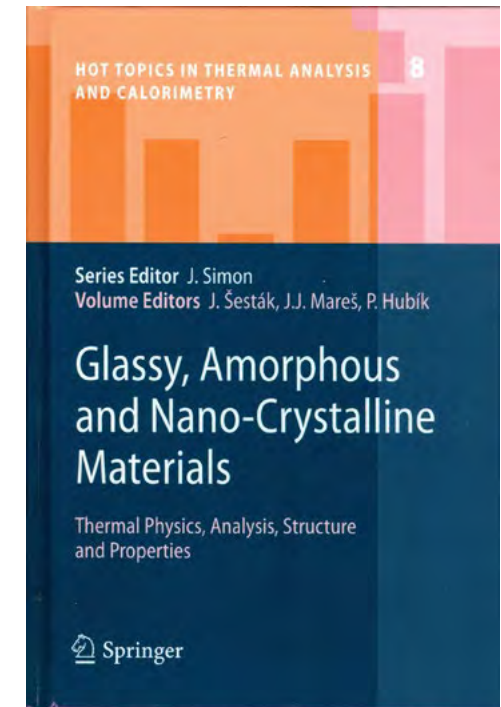


**Fig. 7:** Sample holder for realization of the point contact to high resistance materials enabling one to measure parameters otherwise inaccessible by magnetotransport methods.

Analysis of space charge controlled I-V curves then enabled us to determine required transport parameters and local trap concentrations as well. A similar point contact method was successfully applied to other insulating materials, e.g., to single crystalline intently undoped diamond [13]. Besides universal  $I \sim V^{3/2}$  characteristics (theoretically predicted earlier but observed for the first time by this group) a peculiar de-



**Fig. 8:** Two examples of computable resistance measuring patterns [14]. The left hand one is convenient e.g. for application to highly resistive self-supporting drum-like structures, while the right hand one fits well for quick testing of wafers.



**Fig. 9:** Facsimile of a book [15] edited and coauthored by workers of Department of Semiconductors (in 2013 a total of 8799 recorded chapter downloads).

pendence of charge injection from the point contact on the surface resistivity ( $\rho^{\square}$ ) was discovered. This effect became a basis for a new technique of estimation of surface resistivity in the range  $\rho^{\square} \in (10^{12} - 10^{17} \Omega)$  otherwise inaccessible by standard methods. Of general practical significance also, is a method of resistivity measurement of flat structures based on application of the Thompson–Lampard theorem, a lesser known theorem of 2-dimensional electrostatics. The method which was proved to be dual to the popular van der Pauw technique preserves some of its advantages and can work even in cases where the van der Pauw method fails. Our paper [14] (issued in the compilation of outstanding papers for the 90<sup>th</sup> anniversary of Meas. Sci. Technol. in 2012) among others contains directions on how to design a wide class of computable measuring structures, two examples of which are depicted in Fig. 8.

### Theoretical Achievements

Some of the results achieved in cooperation with the theory group, concerning amorphous state and relevant concepts for its investigation are contained in a book [15] (see Fig. 9), edited and coauthored by workers of our Department. Besides contributions on oxide- and bio-glasses, of more general interest are chapters dealing with quantum periodic chemical reactions, precursor of life processes, and with the concept of hotness manifold, basis of phenomenological temperature. Further results of cooperation





**Fig. 10:** Logo of the fourth Prague FQMT conference held in 2013.

between the transport and theory groups can be found in the proceedings of international FQMT conferences, which deserve special attention.

### Other Activities

The Department of Semiconductors is the principal organizer of the highly recognized series of the international Prague conferences “Frontiers of Quantum and Mesoscopic Thermodynamics” (FQMT) (see Fig. 10, [16]). The series started with FQMT’04 in the summer of 2004. Due to the success of the series, the interval between the events was shortened from four through three years to the current two years. The last two events (FQMT’11 and FQMT’13) were organized in years 2011 and 2013. The FQMT’15 conference is already in preparation [17]. The program committees of the FQMT conferences consist of outstanding scientists including Nobel Prize winners, namely C. Cohen-Tannoudji, S. Haroche, D. Herschbach, A. Leggett, D. Lee, G. ’t Hooft, and F. Wilczek. The Chairman of the organizing committees, V. Špička, and most of the scientific staff of the organizing committees are the members of our department. The typical extent of an FQMT conferences is ~200 people. Within this number many outstanding scientists from all over the world regularly participate, among them the following names are worth highlighting: M. Aspelmayer, R. Balian, G. Baym, I. Bloch, D. Bouwmeester, M. Büttiker, A. Caldeira, N. Gisin, P. Hänggi, H. Frauenfelder, Y. Imry, H. Kleinert, K. Milton, H. Rauch, A. Zeilinger, P. Zöller.

The FQMT conference series is multidisciplinary, addressing the following hot topics: Foundations of quantum physics; quantum measurement, entanglement and coherence; quantum optics; quantum many body physics; non-equilibrium statistical

physics; quantum thermodynamics; dissipation, dephasing, noise and decoherence; macroscopic quantum behavior; Bose-Einstein condensates; topological states of quantum matter and quantum phase transitions; physics of quantum computing and information; mesoscopic, nano-electromechanical and nano-optical systems; biological systems, molecular motors and quantum biology; cosmology, gravitation and astrophysics. Some of these topics are closely related to the scientific interests of members of the Department of Semiconductors, namely, quantum transport in low dimensional and mesoscopic systems. In conferences we thus presented several studies on the theory of open quantum systems out of equilibrium [18], on the quantum transport in molecular systems [19] and on the nature of fundamental physical quantities [20, 21].

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## Department of Spintronics and Nanoelectronics

Molecular beam epitaxy, electron beam lithography, magneto-transport, and magneto-optical laboratories form the experimental basis of the department which together with its theoretical capabilities allow for an extensive research program in the field of spintronics. In a close collaboration with the Charles University in Prague, in the Czech Republic, and Universities of Nottingham and Cambridge in the UK, and by teaming up with a number of other major international research centers in Europe, USA, and Japan, the research of the department focuses on the development of new paramagnetic, ferromagnetic, and antiferromagnetic semiconductor and metal materials for spintronics, new spintronic and opto-spintronic micro and nano-devices, and new quantum-relativistic phenomena observed in these devices. While the frontier basic research plays the central role, the department's vision is also to establish new enabling technologies for future information storage and processing based on electron spin. A co-operation agreement with Hitachi Europe, initially signed in 2006 and renewed in 2011, provides a formal framework for intellectual property protection and for the applied research and development in spintronics.

### Research Highlights

Between 2010–2014, the department has published more than 50 scientific papers including an article in *Science*, 2 articles in *Reviews of Modern Physics*, 17 articles in the *Nature Publishing Group*, and 6 *Physical Review Letters*. Under the Co-operation Agreement with Hitachi Europe members of the department have co-authored 10 patent applications. Among other funding sources, the work has been supported by European Research Council Advanced and Synergy Grants. Below we describe some of the research highlights.

#### Discovery in the Research of Spin-Transistors

Researchers of the department have reported the experimental demonstration of a transistor whose functionality is based on electron's spin [1]. The work was published in 2010 in the **Science** journal and introduced to the general public in the Academy of Sciences press release (25 Dec 2010).

Sixty years after the discovery of a transistor its operation is still based on the same physical principle of electrical manipulation and detection of electron charge in a semiconductor. The technology has focused on down-scaling the device size which has brought transistor dimensions from the original table-top size close to the inter-atomic-distance scale in an astonishingly short time of several decades. Since



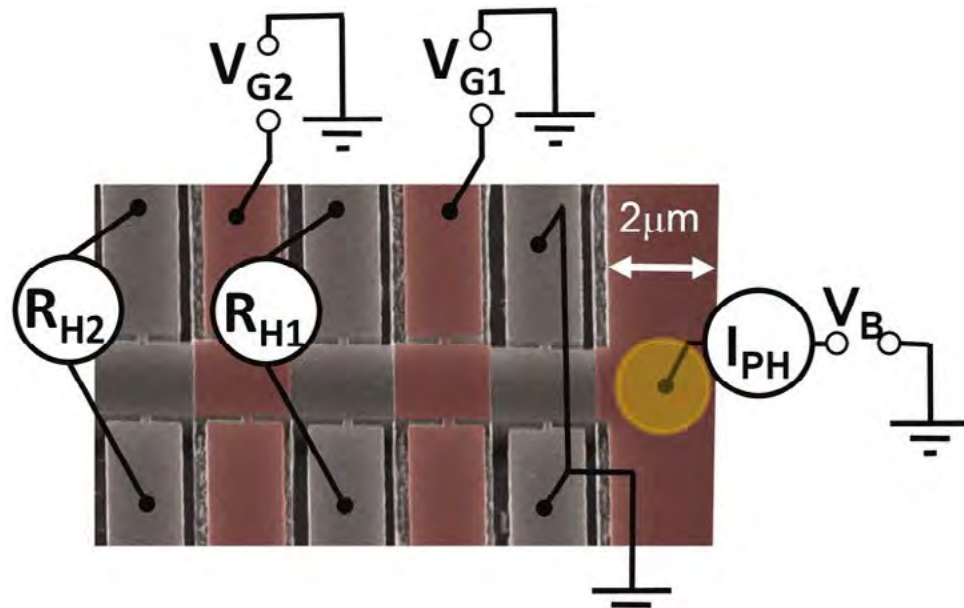


Fig. 1: Electron microscope image of the spin-transistor device

we are quickly approaching the ultimate down-scaling limit it is now an eminent task to establish new physical principles of transistor operation. One extensively studied possibility is to utilize the second basic attribute of an electron which is its elementary magnetic moment, the so called spin.

The theoretical proposal of electrical manipulation and detection of electron's spin in semiconductors is 20 years old. However, its experimental realization turned out to be unexpectedly difficult. The team has recently discovered quantum-relativistic phenomena for both spin manipulation and detection to realize the spin transistor and to demonstrate spin-logic operation.

To observe the electrical manipulation and detection of spins the team utilized a specially designed planar photo-diode placed next to the transistor channel. By shining light on the diode, photo-excited electrons are injected into the transistor channel. In the present work, a circularly polarized light is used to generate spin-polarized electrons. The quantum-relativistic effects are employed to control the precession of spins by input gate-electrode voltages. Quantum-relativity is also responsible for the onset of transverse electrical voltages which depend on the local orientation of precessing electron spins in the transistor channel and represent the output signal.

Whether spin-transistors will become a viable alternative or complement of current electron-charge based transistors in information processing devices is yet to be discerned. Due to the present work this question has turned from theoretical academic grounds to the real world of prototype microelectronic devices.

### Demonstration of a Spintronic Device Based on an Antiferromagnet

Researchers from the department have demonstrated a new principle of operation of a spintronic device based on an antiferromagnet [2]. The work was published in 2011 in the **Nature Materials** journal and introduced to the general public in the Academy of Sciences press release (14 Mar 2011) and on National TV (Milénium, 30 Mar 2011).

Spin, the elementary magnetic moment carried by electrons, represents the basic building block of magnetic materials. It is essential for electronic memory and storage devices, the so-called spintronics. All current spintronic devices used, e.g., in hard drive read-heads or magnetic random access memories are based on ferromagnets. In these materials, like iron or cobalt, spins have a natural tendency to orient in parallel and the materials then act as strong magnets.

There is, however, a much larger family of materials with ordered spins in which spins in the vicinity of one group of atoms in the crystal are oriented in one direction while spins at another group of atoms have the opposite orientation. Besides the large number of these so called antiferromagnets, the materials are attractive because their magnetic behavior is felt only inside the crystal while for the outside world they appear as non-magnetic. They do not produce a magnetic field that would influence the neighboring element which is a particularly useful property when considering the high density of elements in current integrated circuits. It was, however, unknown to scientists on what physical principle a spintronic device, whose active magnetic electrode is made of an antiferromagnet, can operate.

Researchers from the department have introduced not only the principle but also an experimental realization of such a device. When rotating the spins in an antiferromagnetic electrode, the researchers have observed a large change in the resistance of the studied device, comparable to resistance changes in conventional ferromagnetic spintronic devices. The effect is based on a quantum-relativistic phenomenon which, besides its potential for applications, is remarkable also from the perspective of the fundamental research of condensed matter physics systems.

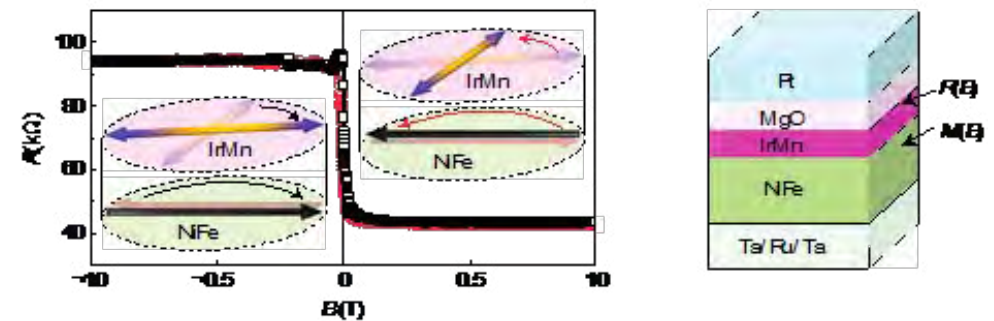
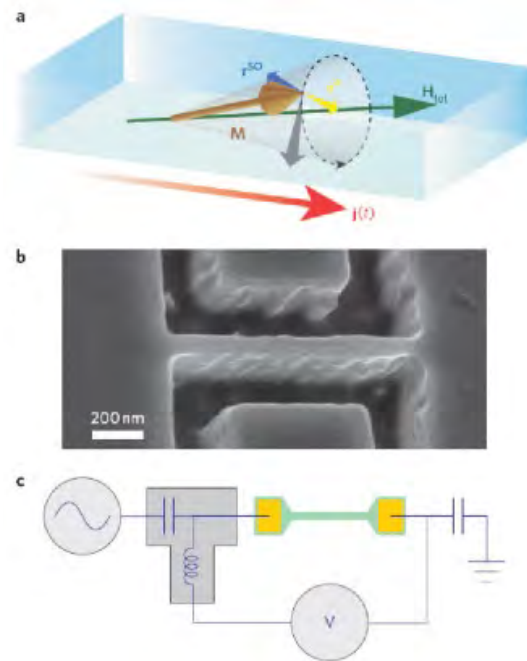


Fig. 2: The measured large change in the resistance upon reorienting spins in the antiferromagnetic IrMn electrode in the new type of a spintronic device

### Discovery of the Relativistic Magnetic Resonance in an Electronic Nanodevice

Researchers of the department have reported that relativistic behavior of electrons makes it possible to utilize magnetic resonance in electronic nanodevices [3]. The work was published in 2011 in the **Nature Nanotechnology** journal and introduced to the general public in the Academy of Sciences press release (30 May 2011).

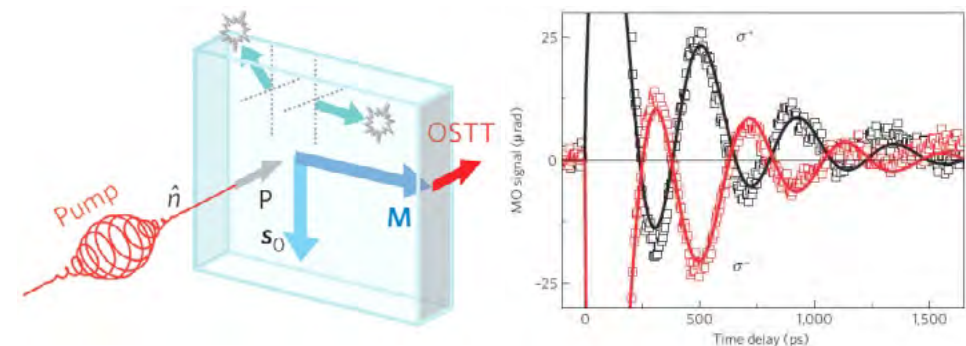
In physics, magnetic resonance represents one of the basic methods for investigating new magnetic systems. With the help of known magnetic elements it is also an indispensable diagnostic tool utilized, e.g., in medicine. The above work introduces a new physical principle of magnetic resonance. The remarkable aspect of the principle is that the driving radiofrequency field is generated and acts directly inside the stud-



**Fig. 3:** The principle of relativistic magnetic resonance, the ferromagnetic semiconductor nanodevice and electrical set-up used for the observation

ied magnetic device, and the device itself serves also as the detector of the induced magnetic oscillations. The researchers have demonstrated that the method allows the performance of detailed investigation of magneto-electronic devices with dimensions of only a few tens of nanometers.

Similar to conventional electronics, spintronics which utilizes both electrical and magnetic properties of electrons in, e.g., new types of memories is approaching the tiny scales of a few hundreds or just tens of nanometers. The relativistic magnetic resonance may become an important tool for exploring and utilizing these ultrasmall spintronic devices.



**Fig. 4:** The physical principle of the optical spin-transfer-torque and the experimental observation of the optical excitation of the ferromagnetic semiconductor by short, circularly-polarized laser pulses allowed by the new phenomenon

### Fast Manipulation of a Magnet by Light

Researchers of the department have reported that a direct transfer of angular momentum from a circularly polarized light to spins allows the excitation of a magnet from its equilibrium state at sub-picosecond time scales [4]. The discovery, enabling the manipulation of spins in a magnet by short laser pulses, was published in April 2012 in the **Nature Physics** journal and introduced to the general public in the Academy of Sciences press release (2 Apr 2012).

Angular momentum transfer from a spin-polarized electrical current to magnetization in a ferromagnet is the so-called spin-transfer-torque phenomenon. It allows, for example, to the writing of information in the latest generation of magnetic random access memories whose development is expected to result in the construction of instant on-and-off computers. The timescales for exciting magnetization by the current induced spin-transfer-torque are nanoseconds. Physicists from the joint *Laboratory of Opto-Spintronics* observed an optical variant of the phenomenon, the so called optical spin-transfer-torque, in which magnetization is excited in a magnetic semiconductor by polarized photo-carriers at timescales which are several orders of magnitude shorter. The material for the experiment was a GaAs semiconductor doped with manganese, which was prepared by atomic layer-by-layer growth. The femtosecond pump-and-probe technique was employed for optically exciting and detecting magnetization dynamics.

The work combines the photo-effect, a phenomenon which is at the very heart of semiconductor opto-electronics, with the spin-transfer-torque which is the key phenomenon for spintronics and magnetic memories. Therefore, it builds a new bridge between these two modern fields of research in microelectronics.





**Fig. 5:** The title page of the special issue of the *Nature Materials* journal on Spintronics

### Spintronics Takes the Center Stage

Researchers of the department have contributed to the 2012 special issue of the **Nature Materials** journal which introduces in a comprehensive format several of the most prominent areas of current spintronics research. The work was introduced to the general public in the Academy of Sciences press release (14 May 2012) [5].

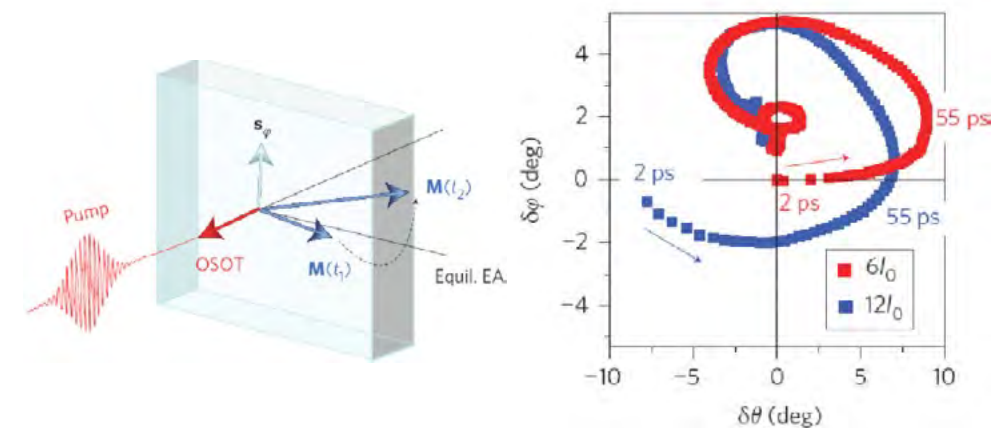
Spintronics is the leading technology for magnetic storage and sensing. In the near future, it is expected to provide high density magnetic random access memories and logic-in-memory architectures, opening a route to the new generation of high-speed, low-power instant on-and-off computers. While the potential for application has been a major driver for the field it would be a fallacy to consider the eventual applications more important than the fundamental insight provided by spintronics research. The spin is a purely quantum-mechanical entity and its interaction with the electron charge or the atomic environment provides a unique opportunity to understand the quantum nature of matter.

### Manipulation of Nanoscale Magnetic Films by Light

Researchers of the department have reported new means for controlling spin by light in semiconductors [6]. The first part of the work was published in 2013 in the **Nature Communications** journal and the second part in 2013 in the **Nature Photonics** journal. The work is follow up to another recent discovery in the field of the manipulation of magnets by light by the researchers from the department published in 2012 in the *Nature Physics* journal. The work was introduced to the general public in the Academy of Sciences press release (22 Apr 2013) and on National TV (Hydepark, 22 Jun 2013).

The preparation of high quality nano-scale films of ferromagnetic semiconductors is a formidable challenge. If successful it would inevitably provide unprecedented grounds for exploring new physical phenomena arising from the interaction of photons with magnets and may suggest new means for the manipulation of magnets in opto-electronic devices at sub-picosecond time scales. Researchers from the department reported the synthesis of prime quality films of ferromagnetic semiconductor (Ga,Mn)As and the discovery of a relativistic effect allowing the manipulation of spins in the nano-scale magnet by short laser pulses.

Electrical current can induce a rotation of the magnetization vector in a ferromagnet due to a relativistic spin-orbit coupling effect and this recently discovered phenomenon is called the spin-orbit-torque. Apart from its intriguing basic physics nature, it is now extensively explored as a new means for writing information in magnetic random access memories whose development is expected to result in the construction of instant on-and-off computers. The timescales for exciting magnetization by the current induced spin-orbit-torque are in nanoseconds. Researchers from the department ob-



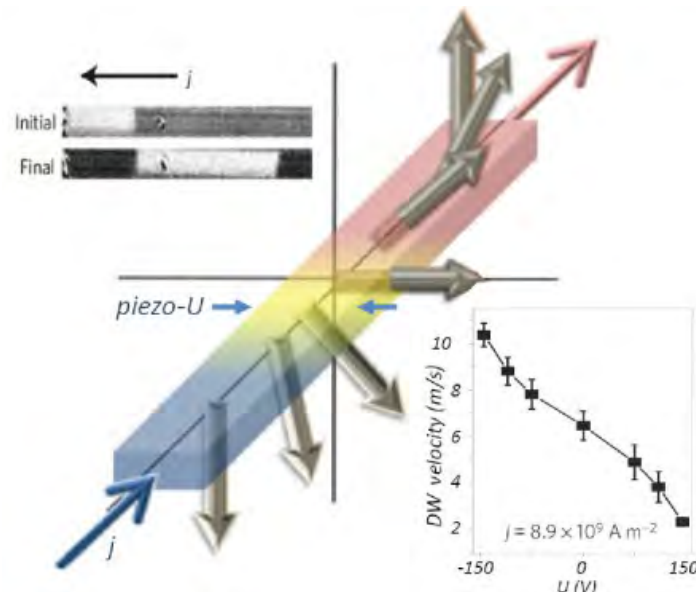
**Fig. 6:** The physical principle of the optical spin-orbit-torque and the experimental observation of the optical excitation of the ferromagnetic semiconductor by short, linearly-polarized laser pulses allowed by the new phenomenon

served an optical variant of the phenomenon, the so called optical spin-orbit-torque, in which magnetization is excited in a magnetic semiconductor by photo-carriers at timescales which are several orders of magnitude shorter.

### An Alternative Concept for Magnetic Memories

Researchers from the department discovered new mechanisms for storing information [7]. The work which reports and explains the origin of a new mechanism that allows electrical control of the velocity of domain walls driven across the magnetic medium was published in 2013 in the **Nature Materials** journal and introduced to the general public in the Academy of Sciences press release (14 Jun 2013).

In conventional microelectronics, information is coded in the electron charge whose value is an universal constant. The electron spin, on the other hand, can be viewed as a microscopic compass whose arrow can point in different directions. In magnetic domain walls, which are used in existing technologies for storing information in magnetic media, the spins point to the north pole on one side of the wall and to the south pole on the opposite side. Inside the wall the spin direction gradually rotates. Similar to the electron charge, the domain wall can be in principle used to not only store but also transport, and process information in a microelectronic device. Its complex and



**Fig. 7:** The internal spin-structure of a domain which is driven by a current in a magnetic medium under an applied piezo-voltage. The top inset shows the magneto-optical microscopy images of the initial and final position of domain walls driven by current pulse. The bottom panel shows that the domain wall velocity can be manipulated by the applied piezo-voltage.

variable internal structure, however, allows for new means to realize these functionalities which are unparalleled in the microelectronics based on the fixed electron charge.

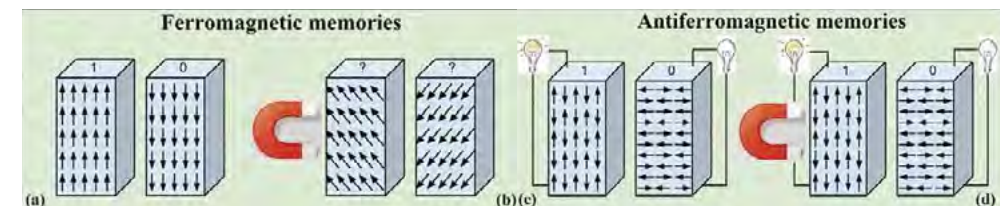
Researchers from the department have focused on the mobility of domain walls driven by current pulses. They placed their magnetic medium with the domain walls on a piezo-electric transducer and demonstrated that the internal structure of the domain wall is sensitive to the applied piezo-voltage. By piezo-electrically manipulating the domain wall internal structure they achieved 500 % variation of the velocity of the domain wall. The experiments have also contributed to a deeper understanding of the microscopic physical mechanisms that allow the movement of domain walls across the magnetic medium.

### Magnetic Inside but not on Outside

Researchers from the department introduced a new concept of antiferromagnetic memories [8]. The work was published in 2014 in the **Nature Materials** journal and introduced to the general public in the Academy of Sciences press release (3 Feb 2014) and on National TV (Události, 12 Aug 2014).

In ferromagnetic materials, information can be stored in “zeros” and “ones” defined by the orientation of magnetic moments, which can be pictured as small compasses (see Fig. 8a). This technology is behind a range of memory applications from kilobyte magnetic stripe cards to terabyte computer hard disks. However, it is dangerous to place a parking ticket or a hard disk next to another magnet or device generating strong magnetic fields because the magnetic moments of the memory can be unintentionally reoriented and the information lost (see Fig. 8b). Moreover, being magnetic on outside, a ferromagnetic bit could disturb a neighboring one if the integration of bits in high-density memories was pushed to limits.

Researchers from the department have demonstrated that it is possible to use another type of magnetic material, the so-called antiferromagnet to store information. Antiferromagnetic materials are magnetic inside, however, their microscopic magnetic moments sitting on individual atoms alternate between two opposite orientations (see Fig. 8c). This antiparallel moment configuration in antiferromagnets, instead of the parallel configuration in ferromagnets, makes the magnetism in antiferromagnets invisible on the outside. It implies that if information was stored in an antiferromagnetic mem-



**Fig. 8:** Ferromagnetic memory (a, b) disturbed by magnetic field and an antiferromagnetic memory (c, d) not disturbed by magnetic field



ory it would be insensitive to disturbing external magnetic fields (see Fig. 8d), and an antiferromagnetic bit would also not affect the neighboring antiferromagnetic bit no matter how densely the bits were arranged in the memory. The outstanding question, however, is how is it possible to read and write information on an antiferromagnetic bit? The answer is in using a special antiferromagnet which changes to a ferromagnet upon heating. To be able to select the magnetic moment direction of the antiferromagnet for encoding “zeros” or “ones” (see Fig. 8c), it is heated up to bring the material into the ferromagnetic phase. A magnetic field pointing along one or another direction is then applied and the material is allowed to cool down back into the antiferromagnetic state where the direction of the antiparallel moments “freezes” (Fig. 8c) along the magnetic field direction applied during cooling. Once in the antiferromagnetic state, the information is written and is no longer sensitive to external magnetic fields. Information is subsequently read by simply measuring the electrical resistance, which depends on the relative angle between the measuring current run through the antiferromagnetic bit and the direction of the antiparallel magnetic moments in the bit (see Fig. 8c).

### Relativity Shakes a Magnet

Researchers from the department demonstrated a new principle for magnetic recording [9]. The work was published in 2014 in the **Nature Nanotechnology** journal and introduced to the general public in the Academy of Sciences press release (4 Mar 2014).

Current technologies for writing, storing, and reading information are either charge-based or spin-based. Semiconductor flash or random access memories are prime ex-

amples among the large variety of charge-based devices. They utilize the possibility offered by semiconductors to easily electrically manipulate and detect their electronic charge states representing the “zeros” and “ones”. The downside is that weak perturbations such as impurities, temperature change, or radiation can lead to uncontrolled charge redistributions and, as a consequence, to data loss. Spin-based devices operate on an entirely distinct principle. In some materials, like iron, electron spins generate magnetism and the position of the north and south pole of the magnet can be used to store the zeros and ones. This technology is behind memory applications ranging from kilobyte magnetic stripe cards to terabyte computer hard disks. Since based on spin, the devices are much more robust against charge perturbations. However, the drawback of current magnetic memories is that in order to reverse the north and south poles of the magnet, i.e., flip the zero to one or vice versa, the magnetic bit has to be coupled to an electro-magnet or to another permanent magnet. If instead one could flip the poles by an electric field without involving another magnet, a new generation of memories could be envisaged combining the merits of both charge and spin-based devices.

In order to shake a magnet electrically without involving an electro-magnet or another permanent magnet one has to step out of the realm of classical physics and enter the realm of relativistic quantum mechanics. Einstein’s relativity allows electrons accelerated in an electric field to order their spins, in other words, to become magnetic. The researchers from the department took a permanent magnet GaMnAs and accelerated some of the electrons inside the permanent magnet by electric field. These accelerated electrons created a new internal magnetic cloud which was able to shake the surrounding permanent magnet, and the researchers detected that the poles of the permanent magnet moved.

### Connecting the Worlds of Semiconductors and Magnets

Researchers from the department realized an efficient spin-charge converter [10]. The work was published in 2014 in the **Nature Materials** journal and introduced to the general public in the Academy of Sciences press release (21 Aug 2014).

Current information technologies are either charge-based or spin-based. Semiconductor microprocessors are prime examples among the large variety of charge-based devices. They utilize the possibility offered by semiconductors to easily electrically manipulate and detect their electronic charge states represented by zeros and ones. Spin-based devices operate on an entirely different principle. In some materials, such as iron, electron spins spontaneously align their direction which generates magnetism. The position of the north and the south pole of the magnet can be used to represent the zeros and ones. This technology is behind memory applications such as computer hard disks. Efficient spin-charge and charge-spin converters are needed for future technologies allowing integration of the so far isolated worlds of semiconductor and magnetic devices.

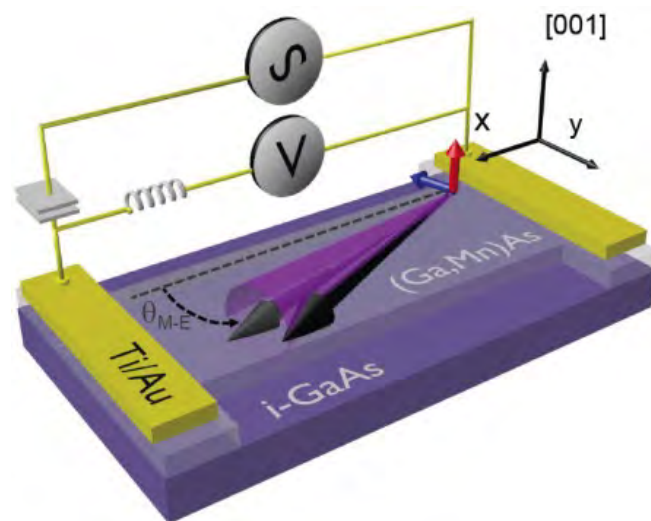
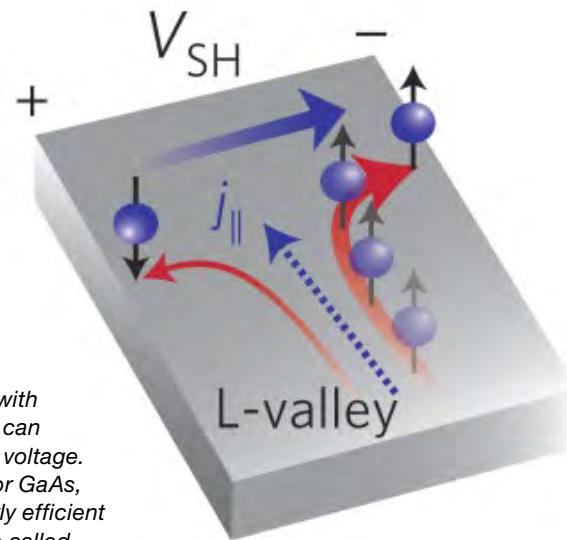


Fig. 9: Schematics of the electrically shaken GaMnAs magnet



**Fig. 10:** Electrons with their spin magnetic moments are deflected to the right or to the left depending on their spin direction due to the spin Hall effect. By this, magnetization of electrons with a preferred spin orientation can be converted into electrical voltage. In a common semiconductor GaAs, this conversion is particularly efficient in one conduction valley (so called L-valley).

Researchers from the department discovered an efficient spin-charge converter in a common semiconductor material GaAs. The device functionality is based on the relativistic phenomenon called the spin Hall effect, which the researchers from the department discovered in 2004 and which since then has become a text-book tool for converting electrical to magnetic signals, and vice versa, in a broad class of metals and semiconductors. So far, the most efficient spin-charge converters have been identified among heavy-metal elements such as platinum. Researchers from the department found that one of the most common semiconductors, GaAs can be turned into an as efficient spin Hall effect spin-charge converter as platinum. They utilized the property of semiconductors in which electrons can carry the current of their charge and spin in different conduction “valleys”. Researchers discovered that by moving carriers in GaAs from one valley to another, the spin-charge conversion efficiency increases in this semiconductor by forty-times.

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## Department of Structure Analysis

Structure analysis is a method for determination of atomic structures of crystalline materials from X-ray, neutron or electron diffraction data. Advanced structure analysis provides information on atomic structures in cases where routine or automatic methods fail. Knowledge of the atomic structure of solids is a prerequisite for any material, chemical, biological and pharmaceutical research.

The Department of Structure Analysis is widely recognized around the world through the structure analysis software JANA which it developed and maintains, and for its training activities in the form of so-called ad hoc workshops. For more than twenty years, the department has been providing worldwide services of advanced crystal structure analysis for almost any kind of crystalline material except proteins. Our team belongs among the few leading groups worldwide, active in the development of computing methods for solution and refinement of modulated or otherwise complicated structures, as well as in the development of electron diffraction tomography and dynamic refinement of crystal structures from electron diffraction data. The latter method is the only means of determining accurate atomic structures of nanocrystals.

The Department of Structure Analysis consists of three research groups: X-ray diffraction, electron microscopy, and the theoretical group. The X-ray diffraction group runs the laboratory of single crystal diffraction, laboratory of powder diffraction, and develops the computing system JANA. The electron microscopy group runs the laboratory of electron diffraction, laboratory of electron microprobe, and develops methods of structure determination from electron diffraction data. The theoretical group specializes to X-ray spectroscopy, electronic structure, magnetism, and calculation of hardness from the first principles.

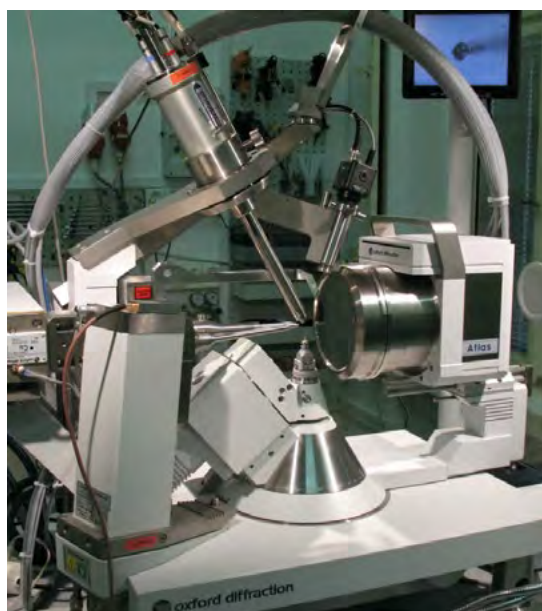


Fig. 1: Single crystal X-ray diffractometer Gemini

## Research Highlights

### JANA2006 – Universal Computing System for Structure Analysis

Structure analysis provides information about the atomic structure of crystals. The structure is calculated from data of X-ray, neutron or electron diffraction. The method of structure analysis from diffraction data is old and mature (this year we celebrate the centenary of the Laue experiment), however it has also many new and attractive branches focused on complicated structures or problematic samples. Two computing systems dominate the field of structure analysis of small and medium structures: SHELX [1] for routine structure analysis and our system JANA (<http://jana.fzu.cz>) for structure analysis of complicated, especially aperiodic, structures. Besides them, several more specialized programs are also used, e.g., FullProf (<http://www.ill.eu/sites/fullprof/>) for analysis from powder data and XD (<http://xd.chem.buffalo.edu/>) for analysis of electron densities.

In 2009 we decided to change the overall opinion that JANA is not suitable for other than modulated structures. From that time the system has offered many more possibilities. Our efforts focused on enhancement of the universal features available in JANA2006, development of user-friendly interfaces and wizards, and changing the overall perception of JANA. During the last five years we organized or participated in almost fifty workshops about JANA with the attendance of about 1000 participants. Tools for routine solution of standard structures have been simplified and integrated to user-friendly wizards while advanced tools for aperiodic, twinned, multiphase and magnetic structures were also greatly improved. Currently JANA2006 can be used for any diffraction data (X-rays, neutrons, electrons), any sample type (single crystals, powders, nanocrystals), and almost any problem of structure analysis except protein structures and calculation of diffuse scattering. The program has 2000 users and 200 citations per year. The development has been closed by a publication [2] summarizing the program features.

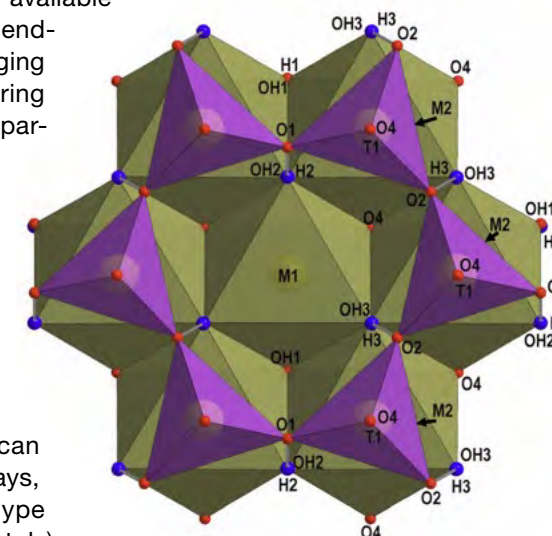


Fig. 2: Atomic structure of the rare layered silicate cronstedtit-1M,  $Fe_{3.54}Si_{1.46}O_9H_4$ , showing geometry of hydrogen bonds  $H...O$  in projection along  $c^*$  axis. T1 denotes tetrahedral sites of silicon partially substituted with iron, while M1 and M2 denote octahedral sites of iron.

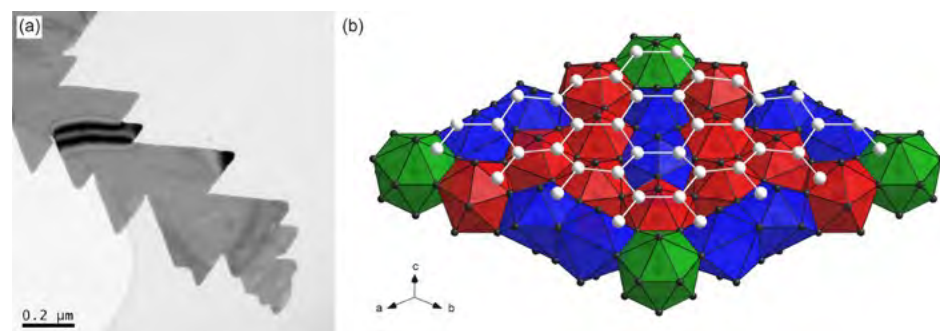
## Where Are Atoms?

### Answering this Fundamental Question with Electron Diffraction

The central question of crystallography is „where are the atoms in the crystal“. X-ray diffraction is a technique almost ideally suited to answer this question and over a million crystal structures were determined with this technique. However, X-ray diffraction is limited by the size of the crystal. X-rays interact weakly with the crystal, and the signal coming from very small crystal (less than about 10  $\mu\text{m}$ ) is too weak to be analyzed. In the current race for smaller and smaller devices and also more and more complicated compounds, the necessity to have large crystal for analysis may be an insurmountable obstacle.

Electrons interact much more strongly with matter, and using a modern transmission electron microscope, diffraction from crystals as small as 10 nm or even less can be recorded. However, in this case strong also means more complicated. Calculations that are easy and fast with X-ray diffraction data are difficult and slow with electron diffraction data. So slow and difficult that using electron diffraction for crystal structure refinement has been for a long time considered impossible for all but the simplest structures.

In 2009 we decided to shift the paradigm and develop a practically applicable procedure for accurate determination of crystal structures from electron diffraction data. This project was a challenge in several ways. While the theory of electron diffraction had been well established, it was by no means clear what was the best way of transferring the theory into a practical system, and if it was possible at all. The development included all steps of the structure analysis – devising the optimal experimental setup, writing software for data acquisition, software for data processing and, finally, developing the method for fitting the structure model to electron diffraction data.



**Fig. 3:** Example of structure solution from electron diffraction: (a) nanoplatelets of  $\text{Cu}_3(\text{SiGe})$  alloy, (b) representation of  $\text{Cu}_3(\text{SiGe})$  structure determined by electron diffraction – slabs comprising of Cu atoms in various coordinations (represented by red, green and blue) are separated by a monolayer of Si/Ge atoms forming a honeycomb arrangement.

We established that a good fit of theory to the data is practically possible only if a special experimental technique called Precession Electron Diffraction is used. In this technique the electron beam is not stationary, but rotates during data acquisition so that it forms a cone with its vertex in the sample. Moreover, to obtain full three-dimensional structural information, a technique called 3D electron diffraction tomography must be used. Similarly to standard tomography, the diffraction pattern is recorded from a number of orientations of the crystal, and combined in a three-dimensional picture of the diffraction pattern.

The most challenging part of the project was the development of algorithms for optimization of the structural model with respect to electron diffraction data. We have the great advantage of being the developers of a general crystallographic computing system JANA2006, in which we could implement the algorithms. To obtain a working system, we combined the crystallographic tools available in JANA2006 with an intensity calculation using the dynamical diffraction theory for electrons. It took several years from the first idea to having a working system. It was a very satisfactory feeling to obtain first structure refinements with the new program and see their quality! The system we produced [3] behaves very similarly to standard structure analysis from X-ray diffraction data. It can be readily used by many crystallographers around the world, which are used to X-ray-based procedures. In short, our method keeps the power, simplicity and ease of use of standard crystal-structure analysis, but brings the scale of accessible crystals sizes down by three orders of magnitude.

## Magnetic Groups and Representation Analysis:

### Competing or Friendly Concepts?

Ordering of magnetic moments in a crystal can be described either by magnetic symmetry or by representation analysis of symmetry properties of the phase transition. The first approach yields magnetic (Shubnikov) space groups while the second one yields a set of possible irreducible representations (henceforth irrep). Both methods are applicable not only to magnetic structures having their translation periodicity identical with the nuclear lattice but also to those being commensurate or incommensurate with the nuclear translation symmetry.

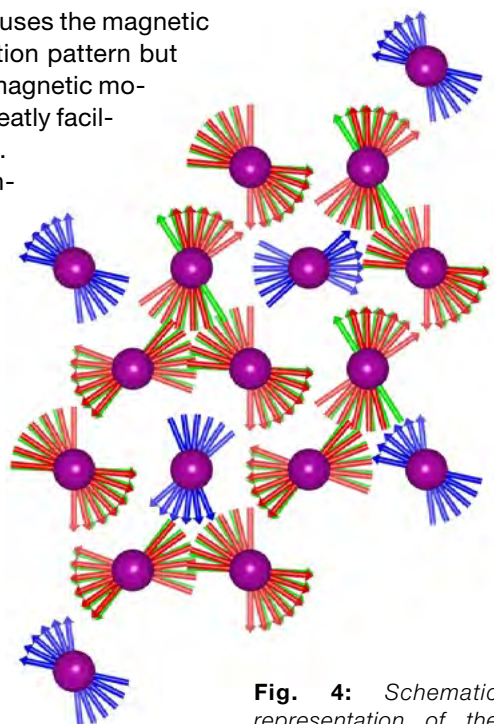
For years representation analysis has been used for the solution and refinement of magnetic structures by the most common computational programs (Fullprof, GSAS). Such an approach might be quite natural for physicists while a crystallographer immediately asks: why such an evident experimental fact as symmetry of the diffraction pattern is not used for the calculation? In the paper [4] we have shown that the actual magnetic (Shubnikov) symmetry can be recognized from the symmetry of the diffraction pattern and that it can be used to merge symmetrically dependent reflection and thus considerably improve stability of the calculation process. In another paper [5] we have shown that this symmetry concept can also be generalized for incommensurately modulated magnetic structures. The door to practical use of the magnetic space and superspace groups has been opened! Our implementa-



tion in the computing system JANA2006 uses the magnetic symmetry not only to handle the diffraction pattern but also to impose symmetry restrictions to magnetic moments in an automatic procedure. This greatly facilitates calculation of magnetic structures.

However, the two concepts of handling magnetic structures are not contradictory. The representation analysis can be used to find a tree of possible magnetic space and superspace groups connected with different order parameters and, therefore, it facilitates determination of the magnetic symmetry. For this reason, representation analysis has been included into the JANA2006 package, too. The procedure is analogical to the method developed by H.T. Stokes and D.M. Hatch [6] and allows an interactive representation analysis for the actual studied structure.

After five years of theoretical and programming work and several successful magnetic workshops the scientific community accepts our concept as the most effective and logical way to calculate magnetic structures. Probably the most interesting among the magnetic structures solved by the new method is the helical screw type magnetic structure of the multiferroic  $\text{CaMn}_7\text{O}_{12}$  with low Cu-doping [7].



**Fig. 4:** Schematic representation of the circular magnetic ordering in  $\text{CaMn}_7\text{O}_{12}$  (view of six unit cells along the modulation vector direction, i.e., the  $c$ -axis). The red and green arrows represent the magnetic moments of  $\text{Mn}^{3+}$  ions located in the Mn1 and Mn2 sublattices.

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## Department of Magnetism and Superconductors

The group conducted experimental and theoretical research focussed on the magnetic, magnetocaloric, thermal and electric properties of novel intermetallics and oxide materials. The scope of **Theory Group's** research was on materials with strong electronic correlations that make physical phenomena unique both from the fundamental and applications point of view. The basic tools were large scale computer simulations in the framework of dynamical mean-field and density functional theories. A large effort was also given to far-infrared magnetospectroscopy, directed both to the experimental and theoretical studies of high frequency vortex dynamics. The **Laboratory of Magnetic Oxides** focused its interest on transition metal oxides, including complex cobaltites exhibiting spin state transitions, materials prospective for thermoelectric energy conversion, and magnetic nanomaterials targeted for medical and biological applications. The research methods of the laboratory comprised an advanced synthesis of the materials, their structural characterization, measurements and analysis of the magnetic, electric and thermal properties. The research of the **High Pressure Laboratory** was concentrated both on experimental studies of intermetallic compounds at extreme conditions and the investigation of novel magnetocaloric materials and corresponding magnetocaloric effects. The scope of the laboratory research included design and construction of the **diamond anvil cell** for direct magnetization measurements under very high pressures.

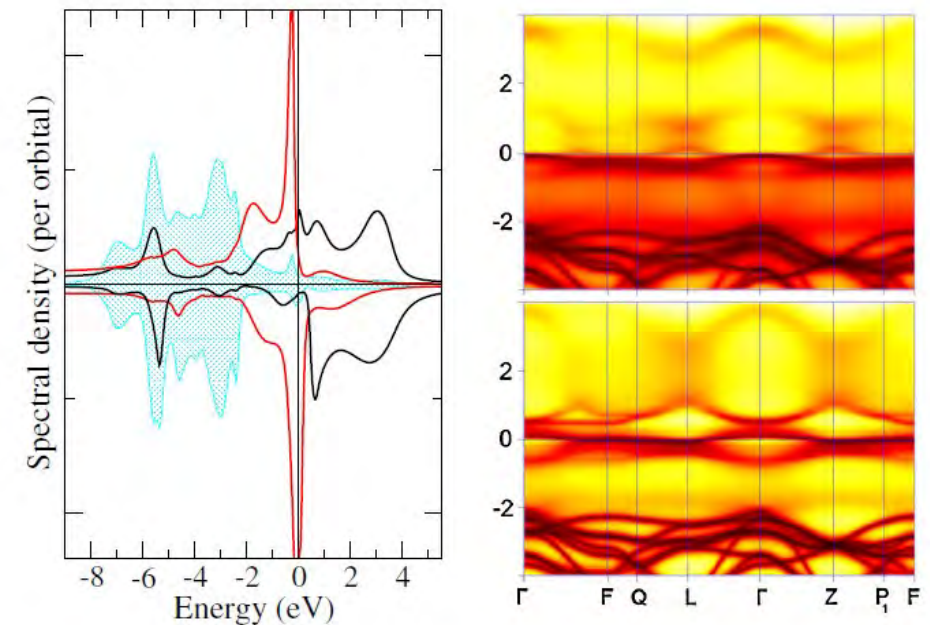
### Research Highlights

#### Theory Group

The work of this group focused on three general topics in the past five years: **spin-state transitions, strong spin-orbit coupling and crystal fields on rare earth ions.**

The **spin-state transitions** were investigated in materials from the  $\text{LaCoO}_3$  family. In a series of dynamical mean-field calculations we were able to reproduce the thermally and doping induced spin-state transitions and explain their microscopic mechanism [1]. The example of the calculated density of states is shown in the Fig. 1. Simultaneously we have studied a much more simplified model of spin-state transition materials – the two-band Hubbard model [2]. We have found that close to the transition the system may become unstable towards long-range order. A particular type of long-range order that can be described as a condensate of magnetic excitons has many peculiar and unexplored properties.

**Spin-orbit** related phenomena have become very popular in the past ten years leading to a great interest in materials with 5d elements, iridium oxides in particular. We have participated in some of the first calculations that provided microscopic un-



**Fig. 1:** On the left, the spectral density of states of the magnetic perovskite  $\text{La}_{0.7}\text{Sr}_{0.3}\text{CoO}_3$ : Co-3d  $t_{2g}$  (red), Co-3d  $e_g$  (black), O p (blue). Right, the same spectral density by symmetry directions in reciprocal space. The upper and lower panels in both cases correspond to two spin projections.

derstanding of the physics of  $\text{Na}_2\text{IrO}_3$  and  $\text{Sr}_2\text{IrO}_4$  [3]. These studies have addressed two basic questions: How does spin-orbit coupling affect the topological properties of the band structures of the studied materials? To what extent are spin-orbit induced Mott insulators similar to cuprate high-temperature superconductors?

In most materials the 4f shells of rare-earth ions couple weakly to their environment. This makes the rare-earth ions unique local probes as their optical or magnetic response carries information about the electronic structure of their surroundings. In order to extract this information one has to know, to great accuracy, the coupling between the rare-earth ion and the rest of the crystal encoded in the so-called **crystal field**. Calculation of the crystal fields from first principles has been a longstanding problem, nonetheless, we have developed a method to calculate the crystal fields and demonstrated its accuracy and capabilities on a series of diverse materials [4].

Addressing new phenomena is intimately tied to the development of new computational methods. There are three developments [5] that stand out in the past five years: (i) Wannier functions with Wien2k, (ii) Bethe-Salpeter formalism for linear response in DMFT and (iii) a new measurement technique in quantum Monte-Carlo algorithm.





**Fig. 2:** *The Far-Infrared Magnetospectroscopy Laboratory.*

The research in the **Far-Infrared Magnetospectroscopy Laboratory** (see Fig 2), was concentrated on study of high frequency vortex dynamics in superconducting materials. Within the COST Action MP1201 we studied high quality NbN films prepared according to our needs. The terahertz thermal spectroscopy measurement was supplemented by a time-domain terahertz spectroscopy method in collaboration with the Terahertz Spectroscopy Group from our Institute [6,7]. An important result, a full quantitative agreement between the experimental data (spanning broad ranges of temperature and frequency) and fundamental BCS-based microscopic theory, was achieved. Our experiments outlined, however, some contradictions in the state-of-the-art theory and thus motivated its improvement [8].

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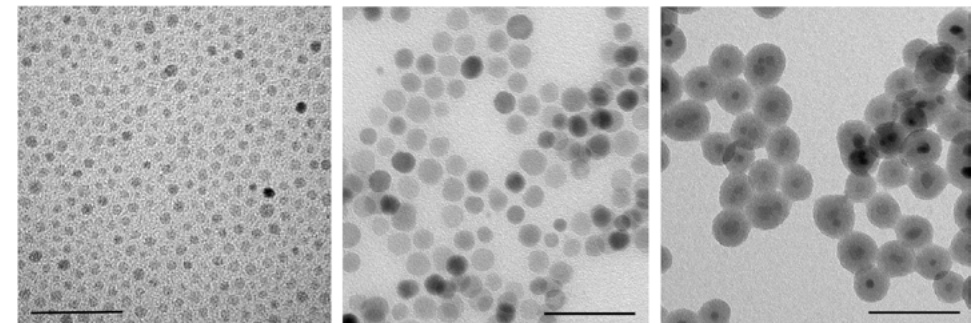
### Laboratory of Magnetic Oxides

The research of the laboratory in the field of **thermoelectricity** comprised both the routes to optimise the thermoelectric oxide based materials for high temperature applications and possibilities of the thermoelectric waste heat recovery from the exhaust gas of automobile engine heat. Due to the lack of commercial thermoelectric characterisation tools which are either unavailable or not trustworthy, we focused essentially on measurement automation and substantial thermoelectric metrology refinement in the evaluation of thermal, thermoelectric and electric power characteristics of materials and thermoelectric modules [9]. This goal was achieved mainly due to a more accurate thermometry and stabilization of the cooling bath. Detail of the measuring apparatus including thermography sensing surface temperature is shown in Fig. 3.



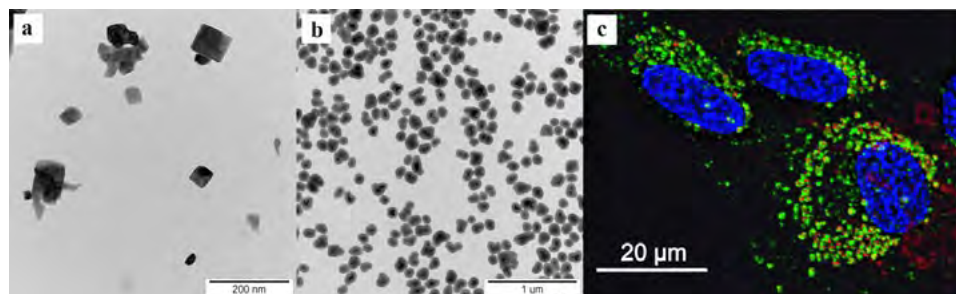
**Fig. 3:** *Automated characterization equipment for testing of thermoelectric modules and materials.*

The interest in **cobalt oxides with perovskite structure** was stimulated by a possibility of the octahedrally coordinated cobalt ions to attain different electronic configurations, characterized as the low, high or intermediate spin states. Numerous cobaltites of  $\text{LaCoO}_3$  type were prepared and their thermally induced spin-state transitions were investigated by experimental and theoretical means. This research included the integral  $\text{Co}^{3+}$  and mixed  $\text{Co}^{3+}/\text{Co}^{4+}$  valence systems based on lanthanum or rare earths – see [10–12]. Special attention was given to the  $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{CoO}_3$  system and some other Pr-containing cobaltites, in which a peculiar metal-insulator (M-I) transition accompanied with important magnetic, thermal and elastic anomalies was revealed. Our specific heat measurements [13–15], supported by X-ray absorption spectroscopy [16] and band structure calculations [17], unveiled clearly that the metal-insulator transition is not due a spin-state transition of cobalt species, as previously speculated, but is associated with significant electron transfer between  $\text{Pr}^{3+}$  and  $\text{Co}^{3+}/\text{Co}^{4+}$  sites. The transition into an insulating state below TM-I thus renders Pr ions into a mixed  $\text{Pr}^{3+}/\text{Pr}^{4+}$  valence and the detailed analysis not only quantified the populations of  $\text{Pr}^{4+}$  states in  $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{CoO}_3$ , but also explained the origin of exchange splitting that took place without obvious magnetic ordering (see also [2]).



**Fig. 4:** *Examples of bare and silica coated cobalt-zinc ferrite nanoparticles possessing different dimensions, the scale bar is 50 nm.*

As regards **oxide magnetic nanomaterials**, major efforts were directed towards finding novel synthetic methods for magnetic nanoparticles and for modification of their surfaces. From the material point of view, the principal studies were dedicated to monodisperse ferrite nanoparticles (Fig. 4) and **nanocrystalline manganites**  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$  in the ferromagnetic range of composition (Fig. 5). At the same time, possible applications of magnetic nanoparticles were analysed, with special regard to labelling and contrast agents for biological research and heating agents for magnetic fluid hyperthermia [18]. Following these aims, magnetic cores were synthesized either in a flux, by sol-gel methods, or via thermal decomposition of metalo-organic precursors, and resulting particles were coated with elaborate fluorescent layers, gold nanoshells, or biocompatible polymer coatings for subsequent biological studies. Importantly, a new method for the synthesis of  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$  nanoparticles with impressive yield was de-



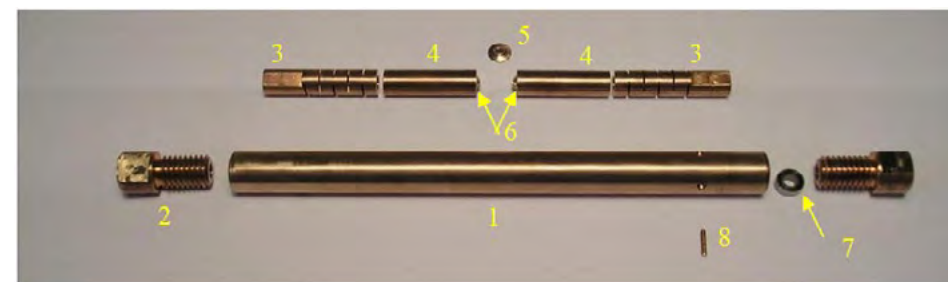
**Fig. 5:** Magnetic nanoparticles  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$  as synthesised in flux (a) and modified with fluorescent coating based on two-ply silica shell (b), which may be observed by fluorescent microscopy (c) showing primary human fibroblasts with nanoparticles (red) localised in lysosomes (green) outside cell nucleus (blue).

veloped using the growth of nanocrystals in the flux of  $\text{NaNO}_2$  at temperatures as low as  $\approx 500^\circ\text{C}$ . An exciting advantage of this simple procedure is the morphology and size distribution of prepared nanoparticles means that they do not require subsequent mechanical processing compared to the tedious preparation via sol-gel [19]. A fundamental question associated with  $\text{Mn}^{3+}/\text{Mn}^{4+}$  ordering in manganite nanoparticles was also resolved based on nanoparticles of “half-doped” systems  $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{CoO}_3$  and  $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ , studied by means of neutron diffraction and precise magnetometry down to low temperatures [21]. Surprisingly, the  $\text{Mn}^{3+}/\text{Mn}^{4+}$  charge ordering and CE-type antiferromagnetic structure characteristic for bulk are completely suppressed when particle size is decreased down to 20 nm, and a ferromagnetic state is stabilized instead. The reason is not in a lower energy of the latter state, but in the hindering of displacive processes through which the charge ordering develops.

### High Pressure Laboratory

Magnetic measurements at extreme conditions represented an essential characterizing tool of the laboratory. Therefore, the design of new **diamond anvil-type pressure cell** was motivated by the need to extend the available pressure range for magnetic measurements. A cell for direct magnetization measurements under very high pressures in the commercial SQUID magnetometer (Quantum Design) was thus designed and built considering: (i) very limited available space (9 mm diameter), (ii) the need to support large forces ( $\sim 10$  kN) necessary for generating the high pressures and the (iii) specific geometric constraints needed to handle the background signal of the pressure cell [22]. The result of this engineering challenge (there are very few high pressure facilities in the world) is shown in Fig. 6.

In the field of **magnetocaloric materials**, the Heusler  $\text{Ni}_2\text{MnX}$  ( $X = \text{Ga}, \text{In}, \text{Sn}$ ) based alloys were considered as prototypical materials for magnetic refrigeration due to the magneto-structural transitions between martensite and austenite phases at about room temperature. The remarkable values of the magnetic properties related



**Fig. 6:** The diamond anvil pressure cell for the SQUID magnetometer: 1) body of the cell, 2) bottom locking nut, 3) springs, 4) piston-guide for the diamond anvils, 5) gasket, 6) diamond anvils, 7) highly polished zirconia ceramic washer with a MoS lubricant, 8) position lock for the upper spring.

to magnetocaloric effect, i.e., the high saturation magnetization jumps and the strong magnetic field dependence of the transformation temperature, were revealed and presented together with high positive values of the isothermal magnetic entropy change. Moreover, magnetocaloric effect in the alloys could be substantially tuned by a variation of composition of the alloy around the off-stoichiometric Mn-rich composition and by an external hydrostatic pressure. In the studied  $\text{Ni}_{50-x}\text{Co}_x\text{Mn}_{30}\text{Ga}_{20}$  alloys, the saturation magnetization of austenite was strongly enhanced with respect to the martensitic one by increasing Co-content and thus the magnetocaloric effect turned from direct into inverse, i.e., a cooling was induced by a putting of the alloy into external magnetic field and vice versa. This possibility to switch the direct into the inverse magnetocaloric effect just by off-stoichiometric variation of the composition of refrigerants gives new application possibilities and opens new way to a novel design of **refrigeration devices** [23–27].

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## Department of Thin Films and Nanostructures

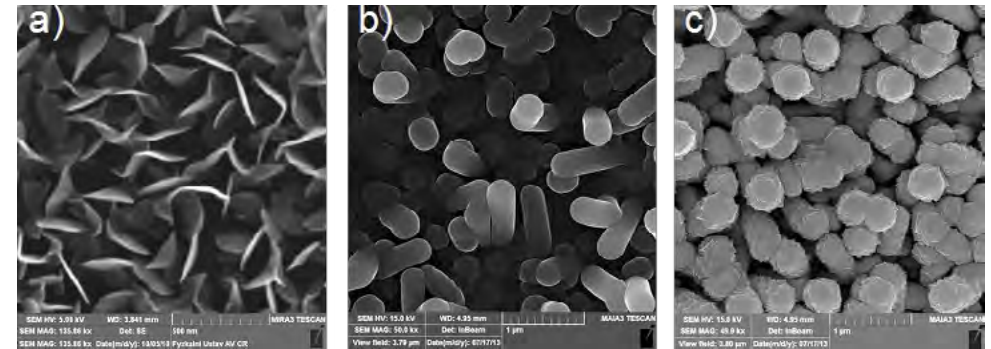
The department comprises four laboratories: Laboratory of Thin Films and Nano-characterization, Laboratory of Silicon Nanocrystals, Nano-surf Laboratory, and Laboratory of Functional Nano-interfaces. These laboratories share many of their research activities as the common target is finding a link between a nanostructure and material properties. The department routinely uses cutting-edge nano-characterization equipment, including various atomic force (AFM) and scanning tunneling microscopes (STM), e.g., combined AFM/STM qPlus (Omicron) featuring high (atomic) resolution or highly stable LHe AFM/STM (SPECS GmbH) for the measurements in temperature ranges from as little as 1.2 K. Measurements in liquids can be performed using AFM NTEGRA Prima (NT-MDT), combined measurement of AFM and Raman spectroscopy (InVia REFLEX by Renishaw) can be carried out using AFM NTEGRA Spectra (NT-MDT) and the systems AFM Dimension 3100 IV (Veeco/Digital Instruments) and AFM Dimension Icon (Bruker) serve for combined measurement of nanostructures and transport properties (conductivity, potential, etc.)

Complementary macro-characterization techniques (conductivity, photoconductivity, the CPM method, Raman and luminescence spectroscopy), together with the technology for sample preparation, modeling and theoretical calculations underpin the activities of the department. The department is staffed by both experienced scientists and young researchers (Ph.D. students), a lot of whom joined the department thanks to the two Centers of Basic Research and the Center of Nanotechnology and Materials for Nanoelectronics. Another characteristic feature of the department is the broad cooperation, both on the international level (e.g., University of Regensburg in Germany; École Polytechnique and CEA Saclay in France; Osaka University and AIST in Japan) and with Czech institutions within the scope of numerous projects (e.g., PolySiMode, GACR Center of Excellence).

### Research Highlights

#### Laboratory of Thin Films and Nano-Characterization

The laboratory is oriented towards the deposition and characterization of nanostructures and thin films based on silicon, in particular amorphous, micro- or nano- crystalline silicon (a-Si:H,  $\mu$ c-Si:H, nc-Si:H). These materials serve as a basis for a new industrial field with an annual production of approximately 50 km<sup>2</sup> of thin films for LCD displays and thin film photovoltaic solar cells. Performance of these devices depends on charge transport properties which are determined by the nanometre structure of Si layer.



**Fig. 1:** Scanning electron microscope images of a) carbon nanowalls (left), b) radial junctions on Si nanowires (center) and c) the radial junctions coated by transparent top conductive oxide. The scales are given in the SEM images.

The nanostructure of  $\mu$ c-Si:H is complicated, with the role of grain boundaries still not completely understood (as discussed in review Mott lecture [1]). Conductive AFM played a fundamental role in the understanding  $\mu$ c-Si:H nanostructure through studies in which we used the tip of an AFM as a local contact for electrical measurements, either in ultra high vacuum (UHV) or in ambient air. Ambient measurements are complicated by the fact that the sample "remembers" previous measurements and repeated measurements lead to different results. In [2] we have successfully elucidated the role of oxidation and we have found a way to achieve results comparable to UHV results even in air.

Surprisingly, the conductive AFM has shown only a relatively small photoresponse to external illumination. In [3] we have shown that this is due to the scattered light of the laser used for registering AFM cantilever position. We have demonstrated a novel way of measurement eliminating this influence and allowing us to measure the photoresponse on a nanometer scale.

The rich variety of forms and properties of nanostructures offer a chance to propose fundamentally new principles of electronic devices, however, this requires investigation of their electronic and mechanical properties. The interest is focused to novel nanostructures, such as nanowalls (e.g., composed of graphene sheets, see Fig. 1a) or nanowires (see silicon nanowires, SiNWs in Fig. 1b, c). The nanostructures are flexible and the tip of the AFM can easily bend or deform them, so the crucial advance was the possibility to use forces as low as several nN or even below. After our first experiments exploring the capabilities of plasmochemical deposition of silicon nanowires [4] we succeeded also in deposition of "lateral" nanowires. In cooperation with École Polytechnique (Paris) we started experiments aimed at detailed characterization of radial junctions on Si nanowires, which are being developed as a new type of solar cells. Our main achievement is the ability to measure the photo response on individual radial junctions on Si nanowires using the AFM tip. We are developing tools for mapping the photoresponse with resolution down to nanometer scale with the aim

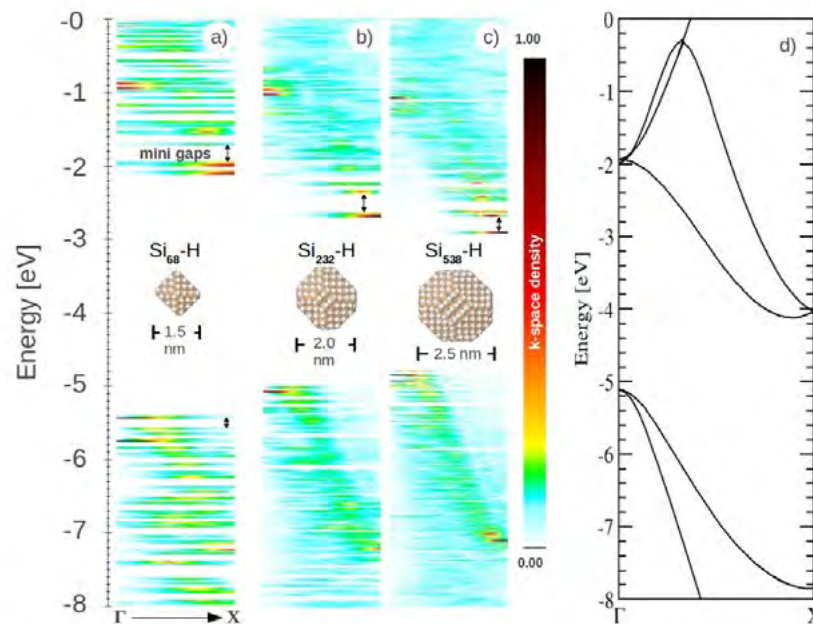


of identifying the weak diodes and thus increasing the conversion efficiency of this new type of solar cells.

### Laboratory of Silicon Nanocrystals

The laboratory is focused on the following problem. Virtually all physicists know that “silicon is a bad light emitter because of its indirect band gap structure”. In spite of this fundamental limitation, there is a constant effort worldwide to make silicon shine; the driving force behind this endeavor is the vision of fusing microelectronics and optoelectronics on a single material basis. Silicon nanostructures, in particular silicon nanocrystals (quantum dots) have been intensively studied during the last 20 years because they exhibit bright luminescence. However, the detailed microscopic origin of this luminescence is still debated. Moreover, fundamentally different views of the electronic band structure of Si nanocrystals can be found in the literature.

Two conflicting opinions do exist: (i) Si nanocrystals retain indirect band gap from bulk silicon, (ii) In nanocrystals generally, as in zero-dimensional (0D) objects, the concept of k-vector and, consequently, also that of electronic band structure (direct/indirect



**Fig. 2:** Energy band structure (*k*-space density) along the  $\Gamma$ -*X* direction of H-passivated Si nanocrystals of different sizes (1.5 nm, 2.0 nm and 2.5 nm) [8]. The subscripts refer to numbers of Si atoms in the corresponding nanocrystals. The right panel shows bulk Si band structure for comparison

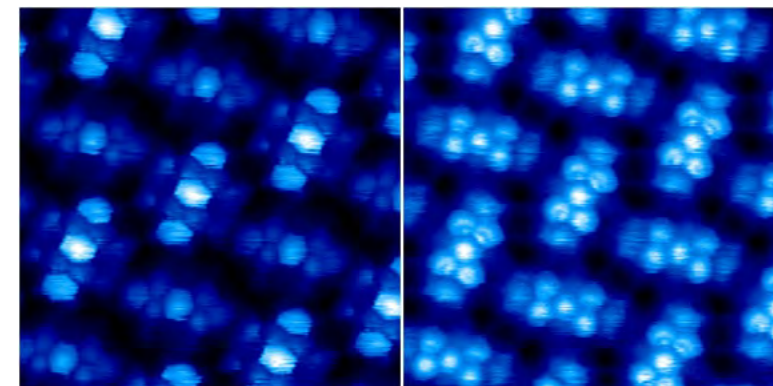
band gap) no longer makes sense. To resolve this puzzle, we have attempted to answer the following three questions: 1) Can the concept of direct/indirect band gap be transferred from bulk material to finite-size quantum dots? 2) If so, do the common silicon nanocrystals (usually 3–5 nm in diameter) possess indirect or direct band gap? 3) If they really inherit the indirect band gap, is there any capability to switch their band gap character over to a direct one?

By combined theoretical and experimental efforts during 2010–2014, we are now able to answer the above questions as follows:

Ad 1) We have adopted the fast local orbital density functional theory (DFT) code FIREBALL [7] to obtain the band structure of finite-size systems. The basic idea of the computational approach consisted in projecting molecular orbitals (obtained using an aperiodic DFT calculation of a nanoscopic system) from real to reciprocal space via Fourier transform [8]. Summary of the results: The principal features of energy band structure in finite-size systems are conserved, but three novel properties occur: (i) minigaps between allowed energy states, (ii) discretization and (iii) delocalization of wave vector *k*. The discretization means that a finite number of *k*-vector values only are now allowed inside the Brillouin zone, and delocalization means that corresponding *k*-values are partially smeared, the resulting band structure being therefore “fuzzy”.

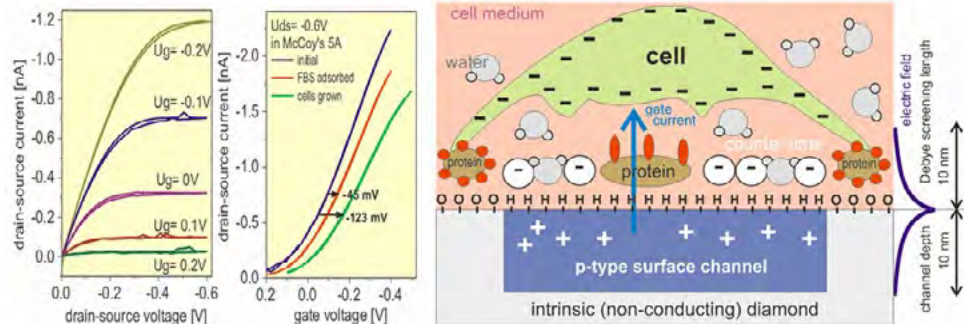
Ad 2) Figure 2 shows the calculated band structure of hydrogen-passivated Si nanocrystals of three sizes 1.5 nm, 2.0 nm and 2.5 nm [8]. The fuzzy character is clearly seen, as well as the fact that silicon nanocrystals keep indirect band gap well below 2 nm.

Ad 3) We have shown, both theoretically and experimentally, that an indirect band gap in ~3-nm Si nanocrystals can be transformed to a direct one via concerted action of quantum confinement and tensile strain [9, 10]. Optical properties of Si nanocrystals thus may compete with those of direct-band gap semiconductors e.g., CdSe or



**Fig. 3:** High resolution AFM-STM images of PTCDA molecules deposited on the Ag(111) surface obtained with Xe functionalized probe with our new LT SPM machine.

### Diamond bio-electronic interface controlled by proteins



**Fig. 4:** Operation and transfer characteristics of a nanocrystalline diamond field-effect transistor with gate immersed in electrolyte with proteins and cells. The gate is insulated solely by hydrogen surface atoms. The characteristics evidence full functionality of such a transistor and sensitivity to changes at the interface with the biological environment. The scheme represents a microscopic model of a diamond-protein-cell electronic interface.

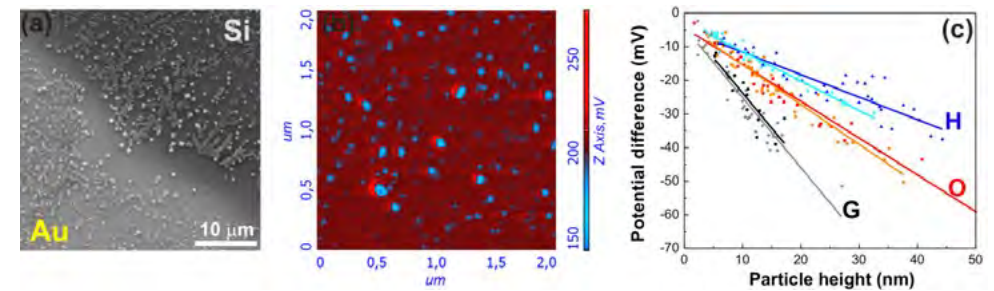
GaAs. The feasibility of band gap engineering in Si nanocrystals (intentional as well as unintentional) was also highlighted in references [11–13].

### Nano-Surf Laboratory

The laboratory aims at understanding and control of mechanical and transport properties of materials and nanostructures on the atomic scale using both experimental and theoretical tools.

In the last two decades tremendous effort has been devoted to the development of new functional nanodevices. Achieving this goal depends on our ability to design, fabricate and control atomic or molecular structures. One of the fundamental problems for further development of nanoscale or few-atom devices is the deep understanding of the charge transport through a chemical bond and its mechanical stability. One of the key questions is: Is there any correlation between the strength of a covalent bond and the charge transport through it? To solve this problem, we devised a rigorous theory establishing the dependence between the chemical force and the current. The theory says that the tunneling current has either linear or quadratic dependence on the force following quantum degeneracy of frontier electronic states. Later, we carried out experimental measurements together with our foreign colleagues, which confirmed the validity of our theory [14, 15].

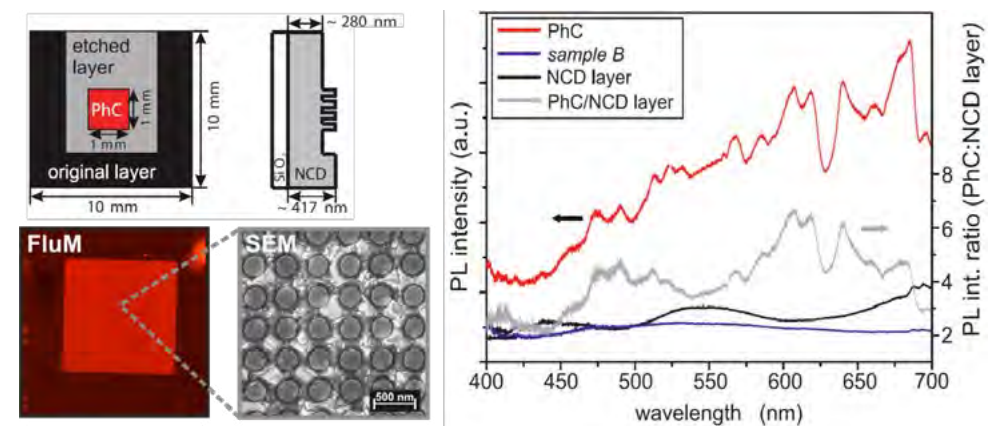
Recently, the high-resolution images of molecules and surfaces acquired by AFM and STM with a functionalized probe amazed the scientific community. The technique became a powerful and widely used tool. However, detailed understanding of the origin of the contrast has not been completely clear till now. We have developed a simple theoretical model, which allowed us to understand in detail all processes important for



**Fig. 5:** SEM image of diamond nanoparticles showing their different secondary electron emission on Au and Si substrates (a). Typical image obtained by KFM of oxidized diamond nanoparticles on Si substrate (b). Difference of electrical potential of nanoparticles on Si and Au substrates as a function of size and surface modification (hydrogenation, oxidation, graphitization) (c).

the high resolution [16]. In addition, the model reproduces experimental results very well. This opens up new possibilities to gain more detailed information about studied systems than just atomic, chemical or electronic structure.

Another important issue for STM is to develop a robust method for the chemical identification of single atoms on a surface. We have achieved the chemical resolution of complex 1D metallic chains grown on silicon surface [17]. Moreover, we were able to resolve different chemical states of given chemical constituents. This initiated our current effort to understand in detail the influence of the nearest chemical environment on chemical activity of single atoms on a surface.



**Fig. 6:** Schematic representation of photonic crystal from nanocrystalline diamond with indicated characteristic dimensions (top). Microscopic image of photoluminescence in the red spectral region and detailed microstructure in electron microscope (bottom). Photoluminescence spectra evidencing significant amplification over a wide spectral region compared to flat or randomly structured diamond layers (right).



In the beginning of the year 2014, we installed a new low-temperature STM with magnetic field, which allows simultaneous detection of force and tunneling current at the atomic scale. This machine opens up completely new possibilities in analysis and control of chemical and physical processes at the atomic scale at cryogenic temperatures, see Fig. 3. We also implemented molecular dynamics with electronic transitions, which allows for very efficient simulations of non-adiabatic processes with several hundreds of atoms. One of the further goals of our group in the near future is to study single-electron charging processes at the molecular and atomic scale.



Fig. 7: Atomic force microscope setup for measurements of proteins and nanoparticles.

### Laboratory of Functional Nano-Interfaces

Research in the laboratory is focused on fabrication and characterization of interfaces and nanostructures based on semiconductor materials (e.g. silicon and diamond), organic molecules and cells. Physical and chemical parameters are employed to control their growth, position and function. Measurement and correlation of structural, (opto-) electronic, and chemical properties on a microscopic level play a fundamental role in constructing physical models of arrangement and functional mechanisms. The main motivation is to understand functionality (such as charge transfer) in such systems with view to perspective applications in energy conversion and biomedicine.

In our bio-electronic research we prepared nanocrystalline diamond microstructures, via surface chemical modification or selective nucleation, that were operational as field-effect transistors or impedance sensors in electrolytic solutions [18, 19]. We used these devices as transducers (and partially also amplifiers) of electronic effects at the biological and molecular interfaces [19, 20]. Grain boundaries were not detrimental; even 100 nm thin devices with 30 nm grains were fully operational [21]. We also developed a novel method that can recognize covalent or non-covalent bonds between organic molecules and diamond by using AFM and/or SEM [22]. Thereby we found that transistor characteristics shift by 50 mV due to a persisting layer of physisorbed proteins. The protein-induced shift is opposite to a common field-effect. We proposed a model whereby proteins replace ions in the close vicinity of the diamond surface and thereby change transfer doping equilibrium (see Fig. 4). The diamond electrodes also enabled real-time monitoring of cell adsorption and growth. These accomplishments led to the award of a L'Oreal Fellowship. We continue this research towards better understanding of cell-diamond electronic exchange during cell cultivation and under gamma radiation.

Our research on nanocrystals and nanoparticles is also promising. By applying electrical current in AFM we created nanopits in silicon thin films and we showed that they can be used as templates for selective growth of silicon and diamond nanocrystals by plasma-enhanced chemical vapor deposition [23]. The process enables direct control of nanocrystal composition, unlike other fabrication methods. Formation of nanocrystals was proved by micro-Raman, conductive AFM, and Kelvin probe microscopy (KFM). By KFM we found that the electrical potential of nanoparticles depends on their size (up to 50 nm), surface chemistry (controlled by hydrogenation, oxidation, and graphitization as confirmed by infrared spectroscopy [24]) and most significantly on the substrate material (see Fig.5). This was independently corroborated by SEM. The difference was up to 0.4V on the same nanoparticles [25]. The potential was also changed intentionally by applying voltage to nanoparticles in AFM. The effect is general as it was observed on diamond and gold nanoparticles. The functionality of nanoparticles must be thus considered always in the context of a particular system. We continue to study the influence on optical and other properties of nanoparticles with various sizes and surface modifications. For that we have developed a unique nanocrystalline diamond photonic crystal that can amplify photoluminescence over a wide spectral range [26].

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## Department of Optical Materials

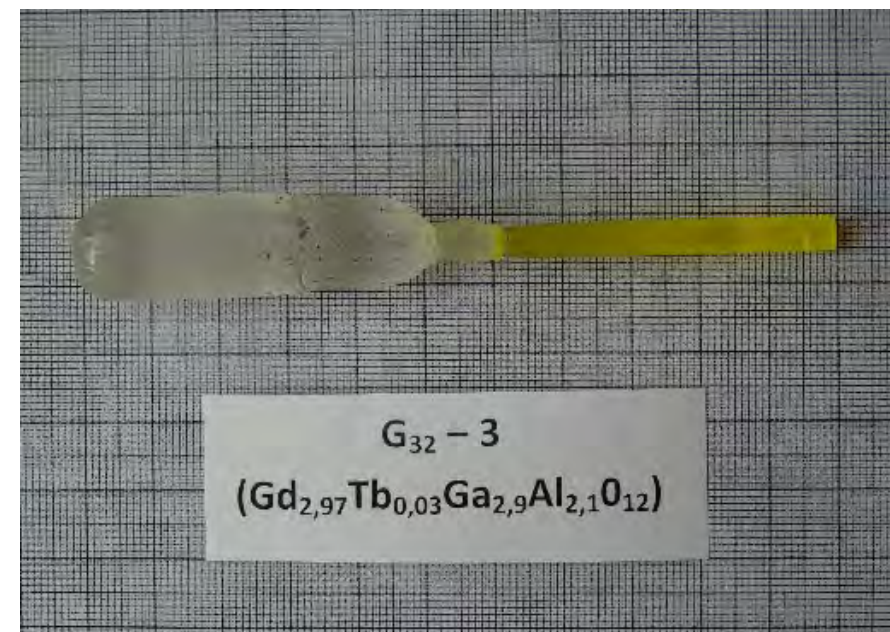
In the department a wide range of functional materials (including composites, glasses, crystalline materials, nanofibers, diamond nanoparticles and biocompatible materials) are prepared using sophisticated advanced technologies (various forms of CVD and plasma techniques, nanospherical lithography, vertical Bridgman growth of halide based single crystals, and phosphate glasses). Their properties are studied theoretically and experimentally by different spectroscopical and optical methods. Theoretical investigations include the nucleation processes, phase transitions and also the kinetic models of luminescence phenomena. In the experiments the specialised spectrometers, such as UV-visible-near infrared absorption/transmission, and Fourier transform infrared, spectrometers, cover a broad spectral range from 200 nm up to 20  $\mu\text{m}$ . for transmittance and reflectance measurements. We use photocurrent and photothermal deflection methods in the study of thin films, time-resolved UV/VIS luminescence and scintillation experiments (X-ray irradiation sources) for powder, film and bulk materials. The convergence of such complementary methods amplifies a cooperative synergic effect between research teams in the department resulting in multifaceted *processing–structure–properties–application interactions*. The long-standing strategy is to allow effective collaboration between particular research teams applying different, but strongly interlinked concepts and methodologies to solve complex interdisciplinary problems with substantial application potential extending from quantum computation processing, advanced sensoric/scintillator techniques to medicine and solar energetics. Given the complexity of material systems and broad portfolio of techniques used for their study we actively collaborate with a few tens of laboratories worldwide which is reflected in the large number of joint publications.

Research activities described below in more details are divided into several groups: luminescence and scintillation materials, chemical vapor deposition diamond and carbon materials, preparation of bulk optical materials, photovoltaics and nanotechnology, electron spectroscopy, and theory of phase transitions.

### Research Highlights

#### Laboratory of Luminescent and Scintillation Materials

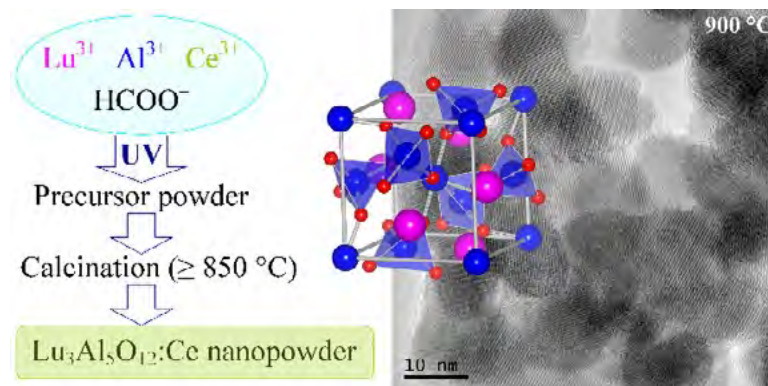
We have systematically studied several material systems based on complex oxides, halides and sulfides. Among the bulk materials the most intensive research and development efforts were devoted to the single crystal garnet scintillators derived from Ce- and Pr-doped heavy aluminum garnet  $\text{Lu}_3\text{Al}_5\text{O}_{12}$  (LuAG). After determination of the scintillation mechanism bottlenecks of this material based on shallow electron traps



**Fig. 1:** Tb-doped multicomponent garnet single crystal grown by Czochralski method in the Chemical Department of the institute.

associated with  $\text{Lu}_{\text{Al}}$  antisite defects the modification of chemical composition was studied as a tool to optimize the material. The gallium admixture appeared effective in shallow electron trap suppression [1]. Furthermore, in collaboration with the group of Prof. A. Yoshikawa at Tohoku University, Japan, using the micro-pulling down crystal growth technology, the combinatorial study within all the group of cerium-doped Ga- and Gd-admixed  $\text{Y}_3\text{Al}_5\text{O}_{12}$  and  $\text{Lu}_3\text{Al}_5\text{O}_{12}$  scintillators resulted in the discovery of a new class of ultra-efficient so called multicomponent garnets [2], where single crystals of  $\text{Gd}_3\text{Ga}_3\text{Al}_2\text{O}_{12}:\text{Ce}$  grown later by the Czochralski method have shown light yield exceeding 50 000 phot/MeV and energy resolution below 5 % at 662 keV. The invited review paper summarizing all these results was published [3]. The absence of lutetium in this crystal host results in the absence of intrinsic radioactivity which enables its usage in a much broader application field. In collaboration with the Chemical Department the Czochralski growth of  $\text{Gd}_3\text{Ga}_3\text{Al}_2\text{O}_{12}$  single crystals with various rare earth dopants has also recently been accomplished in our institute, Fig. 1.

Another optimization strategy of these cerium-doped garnet scintillators has been recently introduced by us in collaboration with the group of Prof. Y. Pan in Shanghai Institute of Ceramics, CAS. It is based on the stabilization of  $\text{Ce}^{4+}$  center by divalent  $\text{Mg}^{2+}$  codopant in LuAG optical ceramics. The stable  $\text{Ce}^{4+}$  center introduces a complementary fast radiative recombination pathway which efficiently enhances the fast part of the scintillation response at the expense of (unwanted) delayed radiative recombina-



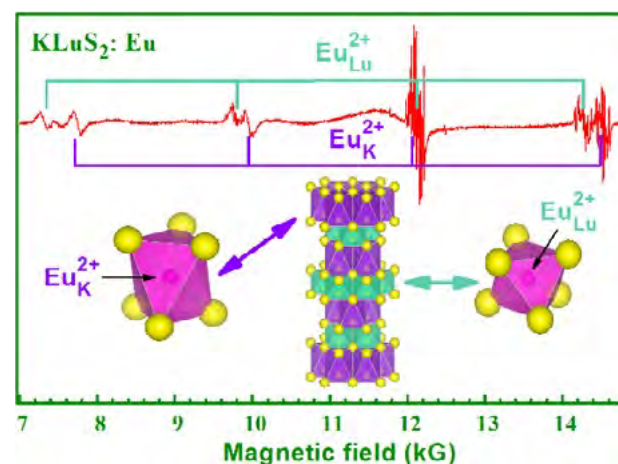
**Fig. 2:** Sketch of the radiation method for Ce-doped  $\text{Lu}_3\text{Al}_5\text{O}_{12}$  nanocrystals. Its structure and HRTEM photograph are displayed on the right.

tion processes [4]. A subsequent study of single crystals of this kind prepared by the micro pulling down technique, provided a deeper insight on the effect of  $\text{Mg}^{2+}$  codopant on all the optical, luminescence and scintillation characteristics in the broad codopant concentration range [5]. Thus, a new optimization tool was found for the whole family of Ce-doped garnet scintillators which greatly improves their practical characteristics.

We have also been studying garnet scintillators in nanocrystalline form in collaboration with the group of Prof. V. Cuba from Czech Technical University in Prague. Using a newly developed radiation method for their preparation, the structurally perfect and well separated nanocrystals of LuAG:Ce were prepared, Fig. 2, which show potential for the application in modern photodynamical therapies for cancer treatment [6].

We also mention our most recent activity in the field of phosphors for solid state lighting: A number of rare earth-doped ternary sulfides  $\text{ALnS}_2$  ( $A = \text{Na, K, Rb, Cs}$ ;  $\text{Ln} = \text{Lu, Y, Gd, La}$ ) were synthesized and their optical and luminescence properties were stud-

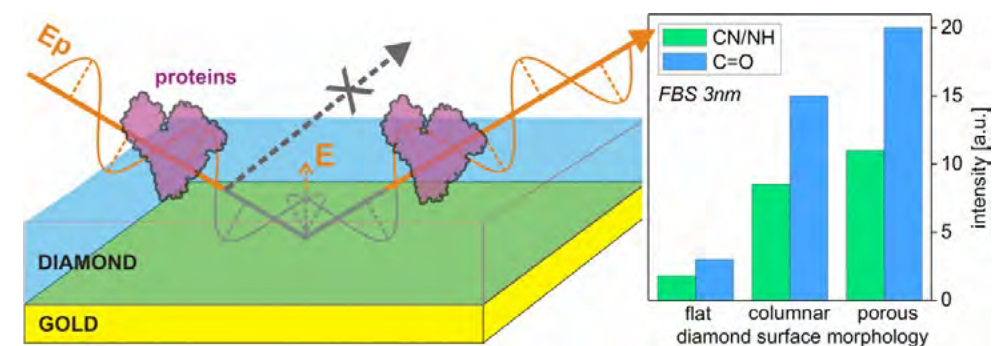
**Fig. 3:** Bottom part – structural units of hexagonal  $\text{KLuS}_2$  and octahedral substituted by  $\text{Eu}^{2+}$  center. Upper part: electron paramagnetic spectra characterizing the  $\text{Eu}^{2+}$  center at  $\text{K}^+$  and  $\text{Lu}^{3+}$  sites.



ied [7], Fig. 3. The most interesting result consists in spontaneous stabilization of the  $\text{Eu}^{2+}$  emission center in these hosts which provides the broad excitation and emission bands in near UV-blue and blue-green-red spectral regions, respectively. A unique feature consisting of tuning the position of  $\text{Eu}^{2+}$  emission over an extremely broad blue-green-red spectral region by chemical composition of these materials [8] shows great application potential for white LED solid state light sources and is protected by Czech national patent [9].

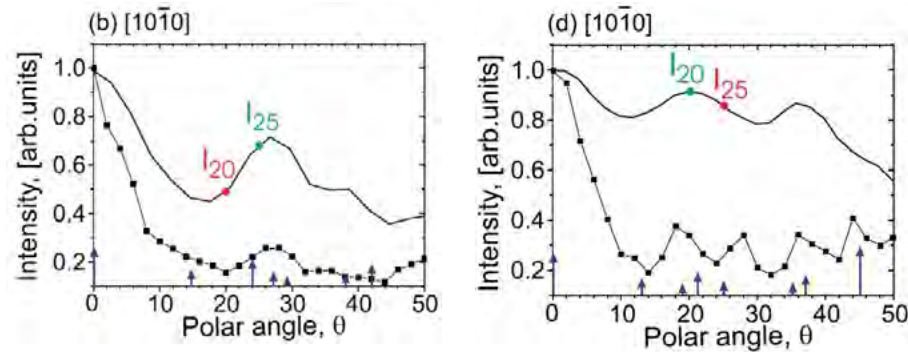
### Laboratory of Diamond Thin Films and Carbon Nanostructures

The core facilities of the laboratory consist of two unique microwave deposition systems: high pressure microwave plasma with ellipsoidal resonator and large area pulsed microwave plasma with linear antennas. Both systems work in a complementary fashion, i.e. low vs. high pressure, low vs. high temperature, large vs. limited deposition area, etc. At the present time, the focused microwave plasma is routinely used for growth of intrinsic diamond thin films. The linear antenna microwave plasma represents the state of the art in the large area deposition of diamond thin films on geometrically complex substrates (drills, implants, rods, etc.). In this system a breakthrough in understanding and technologically controllable growth of nanocrystalline (grain size  $< 100$  nm) and microcrystalline (grain size  $> 500$  nm) diamond films of optical and electronic quality was achieved. We discovered that process parameters such as gas mixture (i.e., mainly adding  $\text{CO}_2$  to the gas mixture  $\text{CH}_4 + \text{H}_2$ ) and process pressure (i.e., the range 6–100 Pa) are crucial for controlling the crystal size and film porosity. Moreover, the chemical vapor deposition (CVD) process is characterized by low temperature plasma ( $T_e < 2$  eV) which allows for plasma assisted CVD deposition at temperatures as low as  $250^\circ\text{C}$ . Thus, the family of temperature sensitive substrates includes glass, gold, silver and germanium. Presently, the deposition system is used for fundamental studies in plasma assisted CVD deposition and plasma functionalization of various



**Fig. 4:** Schematic drawing of the diamond coated Au mirrors and corresponding IR intensities for CN/NH and C=O bonds for flat, nanocolumnar and nanoporous diamond.





**Fig. 5:** Experimental (solid) and calculated (solid with symbols) polar plots of XPD intensities excited from the N 1s level by the MgK $\alpha$  radiation are given for  $[10\bar{1}0]$  direction for GaN(000-1) surface b) and for GaN(0001) d). Vertical blue arrows indicate directions from emitting N atoms to Ga scatters in the GaN crystal. Intensities at polar angles 20° and 25° in b) and d) are the most suitable for crystal polarity determination.

materials for inter-disciplinary oriented fields such as plasma physics (simulation, characterization), opto-electronics (advanced optical elements in IR), material engineering (tailored diamond stress for GaN HEMTs), plasmonics (diamond on gold), photonic crystals (basic research), bio-sensorics (FETs and impedance devices), drug delivery (nanoparticles) and spintronics (diamonds with PL), tissue engineering and regenerative medicine (hierarchically structured films, implants, nanorods, artificial substrates imitating ECM) [10, 11].

The technological progress is demonstrated on the fabrication of optical gold elements coated with diamond films with flat, nanocolumnar, and nanoporous morphologies successfully used for the grazing angle reflectance infrared characterization of fetal bovine serum (FBS) proteins. In spite of the different processing and morphological structures, all diamond samples revealed good stability [12], uniformity, and optical properties, including good reflectivity of the gold mirrors, Fig. 4. Even 3-nm-thick layers of protein molecules adsorbed from FBS solution on the diamond surface were well recognized. The enhanced sensitivity was confirmed for the nanostructured diamond coating. These results are promising for further studies combining optical and electronic monitoring of ongoing electrochemical reactions at the diamond–molecule interface in real time.

The most widely used surface analysis method for material characterization is **X-ray photoelectron spectroscopy** (XPS). Our laboratory is equipped with an ADES 400 photoelectron spectrometer for application of the XPS in the study of solid surfaces. Research activities can be divided into two directions: the first one is dealing with domestic projects and the second one is connected with collaboration activities.

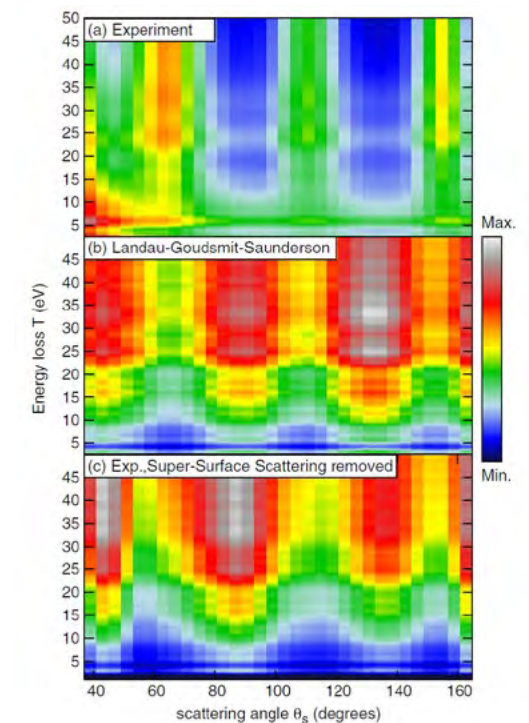
An example of a domestic project is the study on the GaN wide-gap semiconductor problem. GaN has attracted a lot of attention because of its importance for photoelectronics. For device technological process, knowledge about GaN surface polarity, i.e.,

surface termination by Ga or N atoms, is crucial. In our laboratory, a new and very effective method based on the X-ray photoelectron diffraction measurements for determination of the surface polarity was proposed [13]. The suggested simplified approach which utilizes N 1s peaks from two polar angles only for polarity determination. In Fig. 5 the N 1s intensity ratios at polar angle 20° and 25° are different for two GaN surface polarities and, thus, suitable for crystal polarity determination.

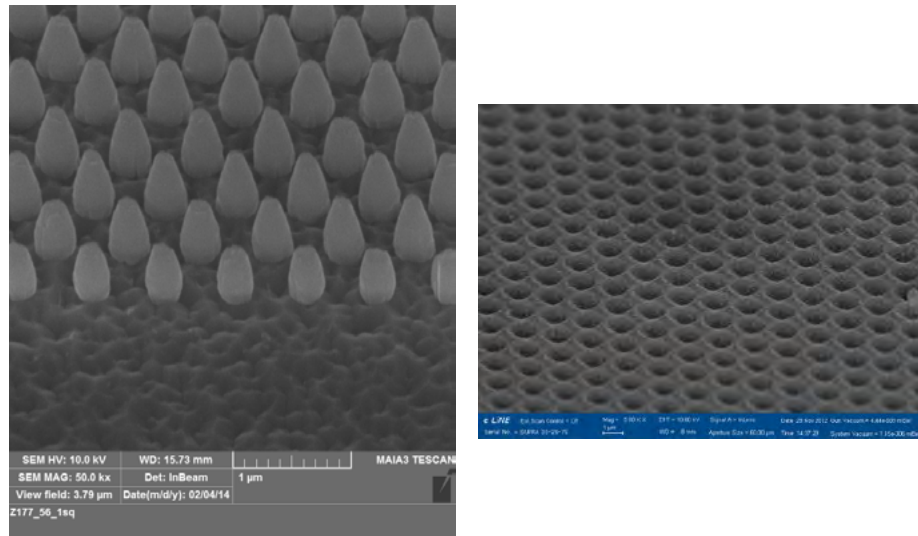
In collaboration with Prof. Werner from the Vienna University of Technology we have measured backscattered electrons from polycrystalline gold samples to verify a new phenomenon predicted by Monte Carlo simulations. This phenomenon was named as super-surface electron scattering [14]. As can be seen from Fig. 6, when the contribution of super-surface scattering is removed from the raw data (Fig. 6a), the resulting spectra, shown in Fig. 6c, are essentially in agreement with the Landau-Goudsmit-Saunders theory, Fig. 6b. The discovered super-surface scattering contributes to our better understanding of electron emission from solid surfaces.

### Photovoltaics and Nanotechnology

The group has been participating in four photovoltaic and nanotechnology based projects of the 6<sup>th</sup> and 7<sup>th</sup> Framework programme of the EU. Optical and photoelectrical characterization of novel (nanostructured) materials for solar cells, as transparent conductive oxides, arrays of ZnO nanocolumns, nanostructured silicon oxides and car-



**Fig. 6:** Combined energy and angular spectrum of 500-eV electrons backscattered from an Au surface. The elastic peak has been removed from all data sets to improve contrast. (a) As measured; (b) Theoretical results according to the Landau-Goudsmit-Saunders theory; (c) Experimental data after elimination of the supersurface scattering contribution.



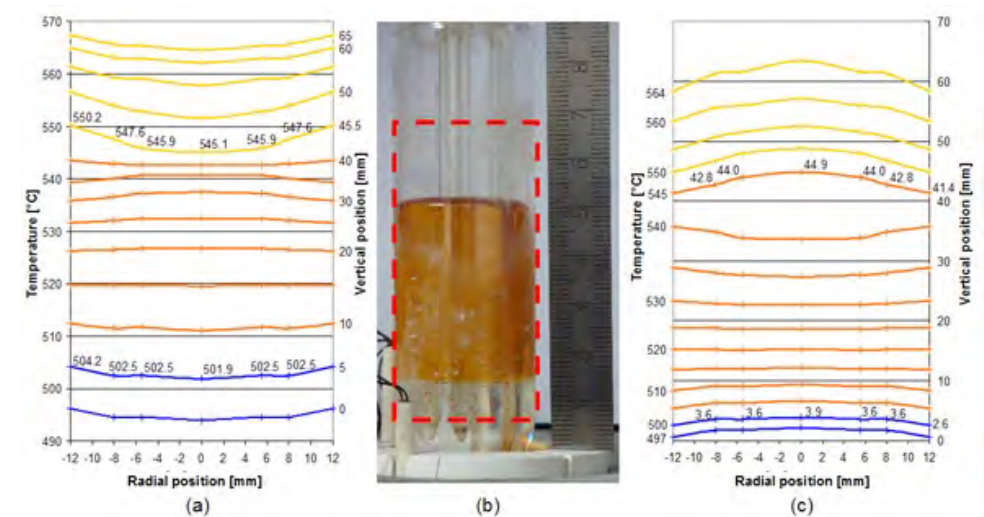
**Fig. 7:** SEM picture, tilted view of nanostructured ZnO substrates for 3D thin film silicon solar cells (hexagonal arrangement of conical ZnO nanocolumns or microholes etched into ZnO layer).

bides was our main task. Our strength lies in our ability to evaluate a low absorbance in thin layers by non-conventional optical and optoelectronic methods, supported by mathematical simulations.

Another task has been connected with our patent application (patent pending in US, EU, China) for a 3-D design of thin film silicon solar cells, as described for example in our joint publication with Oerlikon Solar [15]. This concept creates cells which are electrically thin (to overcome metastability of amorphous silicon) and optically thick (layers about 100 nm thin yield optical absorption corresponding to the much thicker layers). First, we have used a hexagonal arrangement of nanoholes or microholes dry etched into the ZnO front contact layer; amorphous and then microcrystalline Si cells have been “folded into” these holes and covered by a backing ZnO layer, Fig. 7. Analysis, based on our modeling and measurement of optical constants of layers used, points to a possibility to increase efficiency of these cheap thin film silicon solar cells by over 15 %, for the holes depth of about 2 microns. Recently we published our results on alternative 3-D amorphous Si solar cells based on ordered arrays of ZnO nanocolumns. Large scale nano-texturation of ZnO and more conformal coating of the absorbers layers still remains a big challenge for future work.

#### Laboratory of Preparation of Optical Materials and Thermal Analysis

Research work in the laboratory is focused on the search and preparation of materials with promising optical and scintillating properties such as alkali, lead, ternary alkali



**Fig. 8:** Temperature data displayed in radial symmetry as a 2D planar cut measured under stationary conditions at the vertical Bridgman crystal growth (a). Measuring special quartz ampoule filled with lead chloride (b). Its upper yellow-brown part is the molten lead chloride and the colorless bottom part is the crystalline lead chloride. Red dashed line outlines the measured area. Measured temperature data recalculated into isothermal temperature field (c). Areas of different phases are distinguished by different color, i.e., blue for the crystal, orange for the melt, and yellow for the atmosphere over the melt.

lead halides, and rare earth based phosphate glasses. Furthermore, characterization of thermal properties of prepared materials by thermal analysis (TG/DSC, TMA) is performed as well.

The most important results achieved between the years 2010 and 2014 were in the field of crystal growth in our laboratory, through the study of growth conditions (temperature gradient and pulling rate) on the position and shape of the crystal-melt interface when vertical Bridgman growth was performed. At the crystal growth from the melt, the position and the shape of the crystal-melt interface are the key factors determining the final quality of growing crystals [16]. Therefore, a new and reliable method – direct temperature field measurement was designed, developed, and tested during the simulated vertical Bridgman growth with lead chloride used as a model compound. The temperature field was measured by four thermocouples in the ampoule placed at three different positions in two temperature gradients in the furnace and at two pulling rates.

Fig. 8a shows measured temperature data in the quartz ampoule placed in the steep (35 K/cm) temperature gradient. In Fig. 8b, the measuring ampoule pulled out of the furnace with captured crystal-melt interface is depicted. For better understanding of thermal conditions in the system, the measured temperature data were transformed into isotherms using linear approximation (see Fig. 8c). Comparison of the



position and shape of the crystal-melt interface, obtained from the direct observation and temperature field measurements represented by the isotherm 500 °C (PbCl<sub>2</sub> melting point), was the most significant result of the performed study. Details of this study were presented in [17].

Based on these results the crystal growth conditions were adjusted and optimized and single crystals of congruently melting ternary alkali lead halides (RbPb<sub>2</sub>Cl<sub>5</sub>, RbPb<sub>2</sub>Br<sub>5</sub>) were grown by the vertical Bridgman method (Institute of Physics, Prague) and by the micro-pulling-down method [18] (in collaboration with Prof. A. Yoshikawa's laboratory, Tohoku University, Japan). The lead halides and ternary alkali lead halides are studied due to their promising optical properties for applications such as mid IR solid state lasers.

### Theory of Phase Transitions

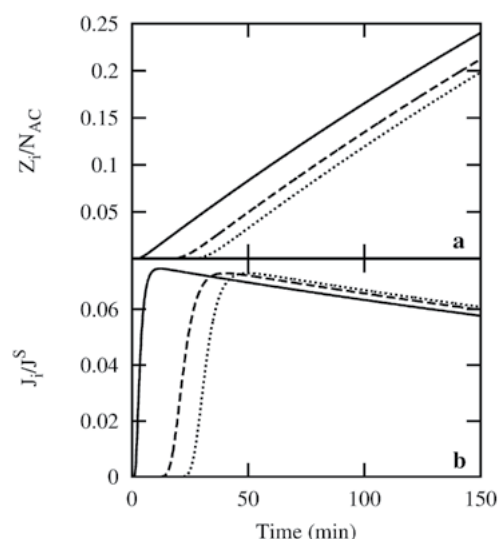
The group studied nucleation and subsequent growth, when stable clusters (nuclei of a new phase) are formed within supersaturated or supercooled parent phases. These stochastic processes determine the final shapes and sizes of crystals, factors governing their resultant physical properties. Basic characteristics of phase transition process, i.e. the size distribution of nuclei, nucleation rate, the total number of supercritical nuclei, and time delay of nucleation, were determined by numerical solution of kinetic equations for crystal nucleation from supersaturated vapor, solution or melt [19-21]. A better understanding of nucleation opens the possibility to explore new approaches to crystallization control.

The nucleation process often occurs preferably on active centers (foreign particles, impurities, surface defects, etc.). On these centers the nucleation barrier is lower and thus heterogeneous nucleation is more probable. In collaboration with Hiroshima Uni-

versity the crystal nucleation kinetics of polyethylene on active centers was studied. Within the context of our model the formation kinetics of the folded chain polyethylene crystalline nuclei at supercooling  $\Delta T = 10.4$  K was analyzed. By the numerical solution of kinetic equations the total number of nuclei, nucleation rate and the coverage of the active centers by the nuclei were determined as a function of time. It was shown that due to exhaustion of the active centers during the phase transition the rate of nuclei formation (after maximum) decreases (see Fig. 9). Such a conclusion will potentially have an interesting impact in polymer-based industry.

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**Fig. 9:** The total number of nuclei scaled by the number of active centers  $Z_i/N_{AC}$  (a) and the nucleation rate scaled by its stationary value  $J_i/J^S$  (b) as a function of time at nucleus size  $i=438$  (full line), 10000 (dashed line) and 40000 (dotted line).



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Institute of Physics  
The Czech Academy  
of Sciences

Division of Optics



The Division of Optics is focused on the research of classical and quantum aspects of the propagation of light, and the research and development of optical structures, materials and technologies. Deep interconnection between theoretical, experimental and technological elements enabled the development, fabrication, and study of a wide range of materials with the specific characteristics covering all research areas of the division. The technology part of the division is mainly focused on research and development of modern optical technologies based on pulsed layer deposition, barrier-torch plasma deposition, dual HIPIMS (High Power Impulse Magnetron Sputtering System), systems with linear hollow cathodes, and low-microwave hybrid plasma. New technologies are also applied for the fabrication of new optical structures and optical components necessary for pioneering experiments in quantum optics and quantum computing.

The research in classical optics is concentrated mainly on holography, the statistical behavior of light beams, and fractal optics. In the area of quantum optics, various types of sources of quantum correlated photon pairs have been designed, and the field of quantum information is focused on the measurement of overlaps, fidelity and purity. Detection of weak and ultraweak irradiation down to one photon, including its characterization together with quantum teleportation and copying is also studied.

The next relatively young research direction in the division is biophysics. In this area the research is mainly focused on interaction of living objects with non-thermal plasma and high gradient magnetic fields.

The division is comprised of four scientific departments:

- Department of Analysis of Functional Materials p. 171
- Department of Optical and Biophysical Systems p. 179
- Department of Low-Temperature Plasma p. 185
- Joint Laboratory of Optics p. 190

and one technical department:

- Optical and Mechanical Workshops Na Slovance

## Department of Analysis of Functional Materials

The scientific work in Department of Analyses of Functional Materials is related mainly to the development of the experimental facilities for the newly oriented interdisciplinary research in the field of advanced functional materials for applications in optics, electronics, optoelectronics and medicine with high innovation potential. The laboratory's focus is schematically shown in Fig 1. These laboratories were financed by the EU Operational Program, Prague Competitive through two different strategy projects of the Institute of Physics: (i) the Centre for analyses of Functional Materials (SAFMAT) and (ii) the Centre for Functional Materials for bioapplications (FUNBIO) over the period 2009-2014. Both centres operate in close collaboration across the Institute of Physics especially with the Departments of; Optical and Biophysical Systems, Low-Temperature Plasma, Thin Films and Nanostructures, Optical Materials, and Functional Materials. Both centers are open to the wider scientific community and the SAFMAT center is listed in the current Roadmap for Large Research, Development and Innovation Infrastructures in the Czech Republic.

In order to successfully develop the scientific program of both of the above mentioned centres, the Department of Analysis of Functional Materials is responsible for the operation of a number of important experimental devices and technologies that are listed below:

- **NanoESCA laboratory:** NanoESCA is a device based on new ideas and a construction connecting a PEEM-Photoemission Electron Microscope with photoelectron spectroscopy for chemical analyses (ESCA). Combination of the methods opens up a possibility to study chemical composition and structural properties with the lateral resolution on the nanometric scale. This point is very important for nanotechnology

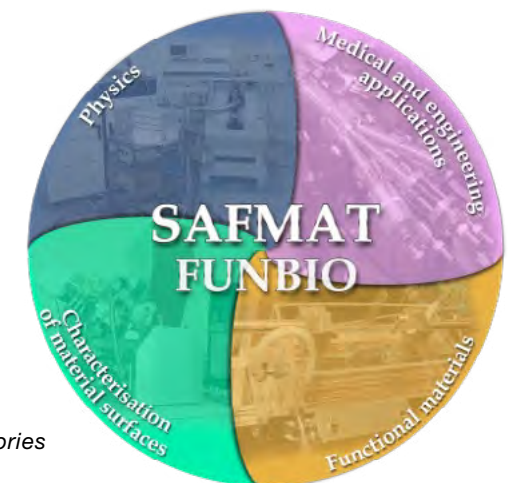
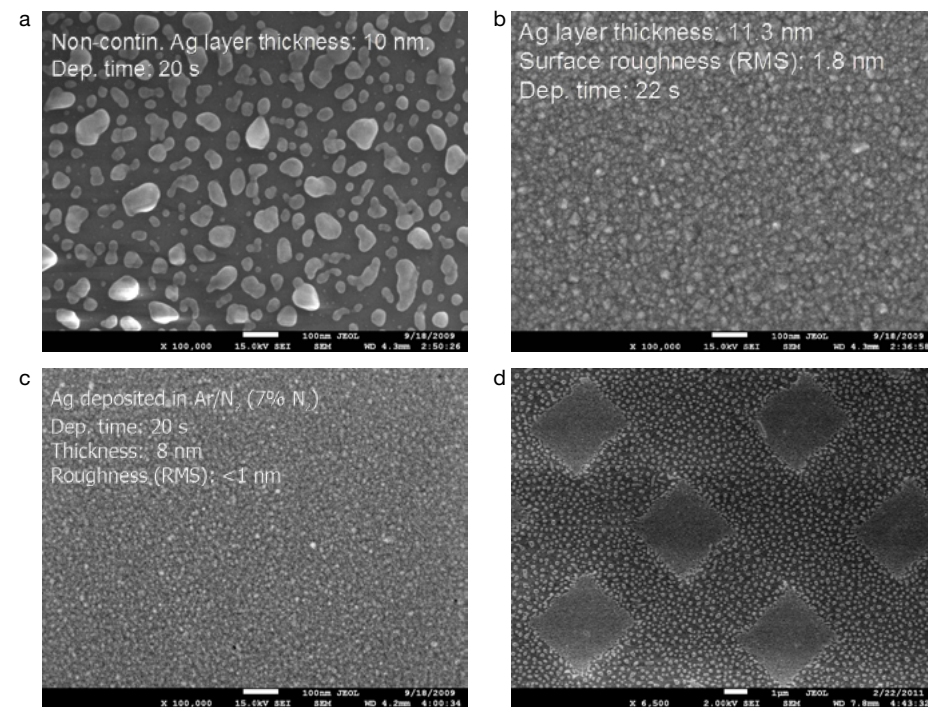


Fig. 1: The research focus of laboratories SAFMAT and FUNBIO

as it allows the complex analysis of a chip. The apparatus is based on the integration of two energy analyzers of the kinetic energy of emitted electrons, filters and the imaging column commonly used in electron microscopy. Three different operating modes use different parts of the electron optics: PEEM microscope, classical ESCA mode and 2D imaging ESCA and PEEM modes.

- **Electron paramagnetic resonance (EPR)** is the spectroscopic method based on the measurement of absorption or emission of electromagnetic radiation (microwave (MW)) by unpaired electrons in the frequency range from a few GHz to 240 GHz. The energy absorption leads to the transitions of the electrons between energy levels, corresponding to different spin orientations of unpaired electrons of atoms or molecules in the external magnetic field. EPR could be used for the determination of structure, dynamics and spatial distribution of paramagnetic objects. This method allows investigation of the local (at atomic level) properties of solid states, liquids and biological



**Fig. 2:** SEM images of surface of Ag thin films growing by magnetron sputtering on fused silica (1285 nm) Si substrates a) non-continuous films with effective thickness “10 nm”; b) the film with thickness 11.3 nm fabricated using a  $\text{AgO}_x$  seeding underlayer; c) ultra-smooth Ag thin film with a thickness of 8 nm fabricated by sputtering in Ar/N atmosphere; d) pattern produced in the 10.8 nm Ag thick film. The square blocks represent the non annealed area surrounded by surface with Ag nanoparticles made by pulsed laser annealing.

objects. The EPR laboratory is equipped with the highest class spectrometer in its category – Bruker ELEXSYS E580, designed to measure electron paramagnetic (spin) resonance in both modes - continuous wave (CW) and pulsed (FT), both in the most common X-band (9.4–9.8 GHz) and in high-frequency Q-band (34 GHz) frequencies.

- **Scanning electron microscope (SEM)** Tescan FERA3 with xenon plasma focused ion beam for nanomanipulation and materials’ study. The apparatus allows the atomic concentration analysis, crystal lattice orientation study and observation in nitrogen atmosphere.
- **AFM for biological applications** equipped with an atomic force microscope (AFM) Bruker ICON for the organic materials surface studies with a glove-box for atmosphere and temperature control. The apparatus will be exploited for example in examination of channel opening in cell membranes interacting with nanocrystals and organomolecules.
- **Infrared spectral ellipsometer** laboratory with an IR-VASE ellipsometer is suitable for nondestructive measurements of optical properties of organic and inorganic coatings in the spectral range 1.7–33  $\mu\text{m}$ . Such experiments allow investigation of optical constants and thickness of coatings as well as their physical properties such as electrical resistivity, concentration of free carriers of charge, phonon structure, etc.

In the field of thin film fabrication by Physical Vapour Deposition techniques, we developed and constructed new technologies for different kinds of coatings and nanostructural thin film fabrications. The attention was focused on the development of hybrid deposition techniques with auxiliary plasma discharges for optical, magnetic and organics films. In our research we do not want to use one deposition technique, for example magnetron sputtering, for fabrication of some specific coatings. The scientific idea in our PVD laboratory is to find the best methods to fabricate the films and nanostructure with the demanded structural and functional (luminescence or magnetic) properties for particular physical and technological problems.

The next direction of research is focused on cooperation with partners from Charles University on the operation and development of a *Materials Science beamline* (MSB) located in Synchrotrone ELETTRA in Trieste. MSB is an open access laboratory and represents a multi-purpose beamline suitable for experiments in a field of surface science, material science and physicochemical interactions of organic molecules with solid surfaces.

## Research Highlights

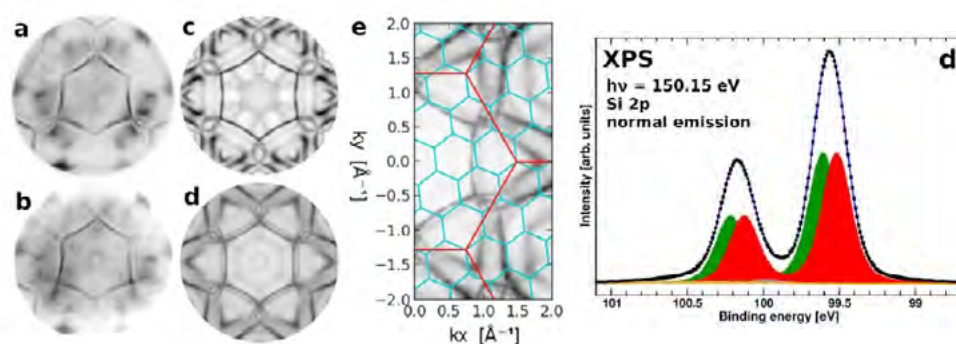
### Ultrathin Metallic Films and Nanostructures

A considerable number of metal-dielectric devices use ultra-thin noble metal (Ag, Au) layers. For instance, colour reflecting structures exploit a localized plasmon resonance of a nano-island metal layer in combination with interference behaviour of dielectric



coatings. Another class of stratified optical devices requires an ultra-thin continuous noble metal layer. The typical optical metal-dielectric devices are transmission induced filters or conductive transparent multilayer structures known as “a transparent metal”, which consists of a multilayer stack of multiple resonators. Silver exhibits a great potential for fabrication of metal-dielectric transparent conductive coating due to its unique optical constants and excellent electrical properties. The nanostructure of the Ag layer is mainly influenced during the initial stage of the silver nucleation. Therefore, we focused our attention on studying the initial stage of the nucleation and the layer growth by optical monitoring by means of in-situ spectral ellipsometry. The main goal of our complex research was to develop targeted influence on the growing regime of the thin films fabricated by magnetron sputtering for different kind of applications. The non-continual growth mode of the layer nucleation was clearly distinguished in Fig. 2a. We proved, that the nucleation mode and the resulting nanostructure can be significantly influenced either by an ultra-thin silver oxide interlayer Fig. 2b [1] or by the using an Argon/Nitrogen working gas mixture Fig. 2c [2].

After the fabrication of Ag ultrathin and smooth films the next logical step was the Ag The laser interferometry patterning represents advanced modification of the described method. Our ultrathin silver films were patterned by means of pulsed laser. Laser irradiation is carried out through phase masks forming parallel fringes – see Fig. 2d. They are projected onto the samples by means of two lenses in a telescope configuration leading to a reduction of their period. This configuration can produce a periodic structure consisting of alternate areas containing NPs and continuous metal film with a period down to few micrometers. The resulting structure combines plasmonic and diffractive optical properties [3]



**Fig. 3:** Angle-resolved photoemission  $k$ -space maps of (a) clean Pt(111) and (b) Si- $(\sqrt{19} \times \sqrt{19})R23.4^\circ$ /Pt(111) surfaces at the Fermi level. DFT-calculated band maps for the best-fit model at first (c) and higher (d) BZ (e) Map of the first two BZ of the (1x1) (red) with the Si- $(\sqrt{19} \times \sqrt{19})R23.4^\circ$  (blue) Brillouin zones. Panel (d) shows the photoemission doublet Si-2p fitted with two equivalent components supported the best-fit model.

## Surface Characterisation and Electron Structure of Functional Materials

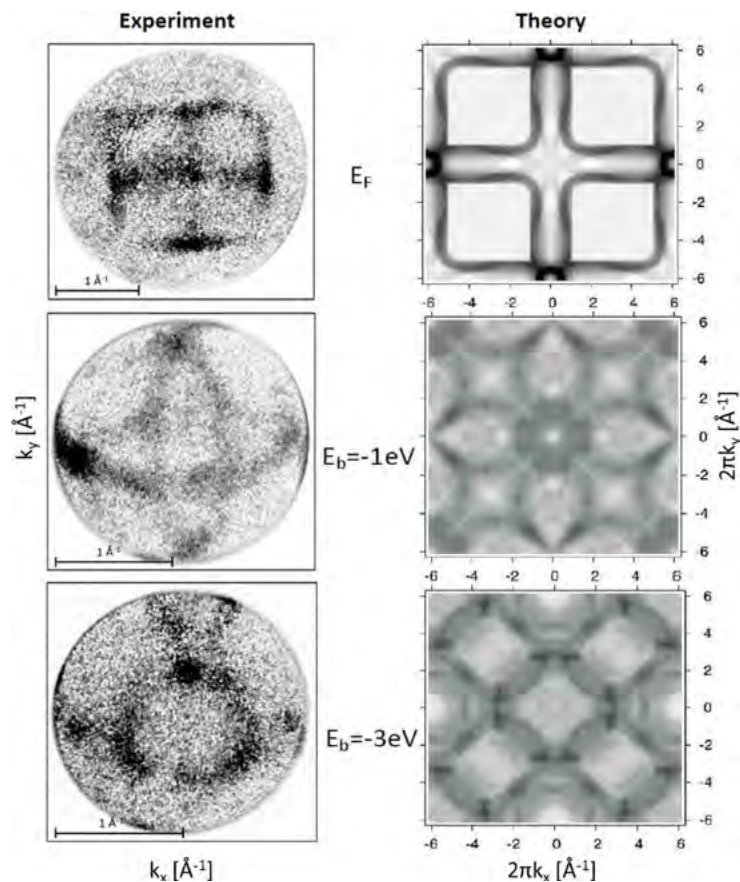
One of the most interesting operational modes of the NanoESCA apparatus is the angular imaging of the photoelectron emission (ARPES). In fact the detection of the angle-resolved photoemission enables mapping of the electron states in the  $k$ -space. Dispersion relations  $\mathbf{E}$  vs  $\mathbf{k}$  are monitored using equienergetic cuts over all  $\mathbf{k}$  vectors from the first Brillouin zone. The  $k$ -space images are acquired with the two instead of three lenses column. It could be considered as a diffraction mode. The cuts are taken with the 0.1–0.2 eV energy resolution and are integrated in the real space area  $\approx 3\text{--}4 \mu\text{m}$  in diameter. Application of all operating NanoESCA modes – PEEM, ESCA and Angular imaging provides an efficient way to select a particular topological feature at a surface, to follow it with full chemical analysis and experimentally to determine its corresponding electronic structure. The investigation of 2D materials such as silicene and graphene, a topological insulator for example BiSe and BiSeTe and Heusler alloys were the main scientific tasks in NanoESCA laboratory.

### Silicene

Alternative advanced synthetic 2D materials to graphene would be silicene and germanene. Up to now, their existence was not proved and research of many labs is directed in this area. The research in the field of characterization of silicone was done in the collaboration with Department of Thin Films and Nanostructures. The panel a) of the Fig. 3 shows the electronic structure of the clean Pt(111)-(1x1)surface with a hexagonally-shaped s-like band crossing the Fermi level and weak features spreading from the center of the Brillouin zone (BZ). The changes of the electronic structure of the Si- $(\sqrt{19} \times \sqrt{19})R23.4^\circ$ /Pt surface is shown in the panel b). The visible changes are found around the center of the BZ. The experimental data imply a very similar chemical environment for all Si atoms and their strong hybridization with the Pt substrate. The STM image (Fig.3c) displays a negligible height difference, indicating that Si atoms are embedded in the Pt(111) surface. Calculation of the Si atom triplet binding energy observed in a protrusion gives a value 52 meV. It is in good agreement with the core level shift 90 meV found in the photoemission Si-2p doublet (panel d) measured at the MSB Czech beamline in synchrotrone ELETTRA in Trieste, Italy [4].

### Heusler and magnetic shape memory alloys

$\text{Ni}_2\text{MnGa}$  Heusler alloys are studied intensively both from the applied and from the fundamental physics point of view. Single-crystalline  $\text{Ni}_2\text{MnGa}$  exhibits the magnetic shape memory (MSM) effect, or more precisely, magnetically induced reorientation resulting in a giant field-induced strain. The existence of the MSM effect and/or giant magnetic field-induced transformation ranks this material among the smart materials. We focused our research on an experimental and theoretical electronic band structure study of slightly Mn-rich  $\text{Ni}_2\text{MnGa}(001)$  crystal surfaces in their cubic austenitic phase. Weakly off-stoichiometric, Mn-rich compounds exhibit the martensitic transformation above room temperature, and consequently they can exhibit the magnetic shape

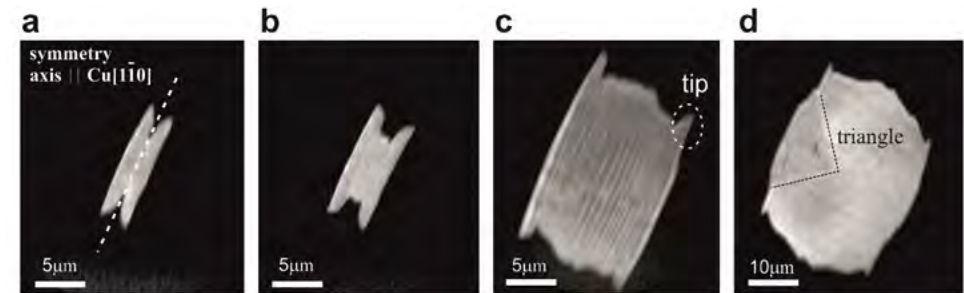


**Fig. 4:** Selected experimental (left panel) and theoretical (right panel) ARPES images of the single crystal  $Ni_{49.7}Mn_{29.1}Ga_{21.2}(100)$ .

memory effect at room temperature, which is of interest for many kinds of applications. We performed the  $k$ -space mapping at the position chosen in the real-space imaging mode, using a He-I discharge lamp. The arrangement of the lenses and apertures in the column transmits a large angular range and it usually covers the first Brillouin zone or more. The quality of the surface of fabricated monocrystal was monitored by LEED and classic ESCA mode of the NanoESCA system. We find excellent agreement between experiment and theory in the energy bellow Fermi level for  $\mathbf{k}$  vectors in the first Brillouin zone BZ as is shown in Figure 4 and presented in [5].

### Graphene

Graphene, a simple two-dimensional honeycomb arrangement of  $sp^2$ -hybridised carbon atoms, is hailed for its exceptional electronic environment. The exceptional elec-



**Fig. 5:** Anisotropic growth of graphene nuclei. (a) - (d) PEEM images of graphene nuclei at different stages of growth, from 2 to 30  $\mu\text{m}$  width (faint hexagonal patterns are artefacts from the channel plate detector). All islands obey a twofold symmetry axis parallel to the fundamental  $\text{Cu}[110]$  direction indicated by the dashed line in (a). Characteristic tips at the four extremities of the islands indicated in (c) are already visible at the earliest stage. Within the largest island in (d) a high-symmetry triangle is faintly visible which – as we will show in dark field contrast measurements – is due to the formation of a well-defined rotational graphene domain.

tronic properties of monoatomic thin graphene sheets triggered numerous original transport concepts, pushing quantum physics into the realm of device technology for electronics, optoelectronics and thermoelectrics. The CVD grown graphene islands on copper foil were analysed by [6]:

- Electron backscatter diffraction (EBSD) data was acquired with an EDAX camera and software on a Tescan FERA 3 instrument. For atomic force microscopy (AFM) a Bruker Dimension Icon was employed. Both EBSD and AFM were performed under ambient conditions.
- at UHV conditions after thermal annealing or ion bombardment by LEED, XPS and  $k$ -PEEM measurements using an Omicron NanoESCA instrument

We were interested in understanding the local influence of the faceting process on graphene growth at the earliest stage. Fig. 5 shows typical small graphene islands, ranging from a few  $\mu\text{m}$  to about 30  $\mu\text{m}$  in width. They appear bright against the dark copper oxide background due to the work function contrast in the energy filtered PEEM imaging mode. All islands obey a two-fold mirror symmetry, and their elongation along an axis oriented parallel to the  $\text{Cu}[110]$  direction reflects the fundamental symmetry of the faceting direction. They exhibit a characteristic tip-shaped protuberance at the four extremities, and already host the characteristic roof-top modulation structure on the micron scale. The investigation of graphene has proved the high potential of the described SAFMAT laboratories for characterisation of functional materials.

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## Department of Optical and Biophysical Systems

The Department of Optical and Biophysical Systems is mainly focused on the research and development of optical materials for micro-electronic, optoelectronic and biomedical applications. The main technique used in this department for optical study of materials is ellipsometry. This technique enabled us to investigate the complex refractive index of materials over a wide spectral range giving access to information on other fundamental physical parameters (crystalline structure, polarization, surface roughness, etc.). The ellipsometry laboratory is equipped with a temperature dependent ellipsometry system allowing study of optical properties of nanostructures, surfaces, and thin films; detection of surface, bulk and interface phase transitions; study of the dynamics of biological films and surfaces, and nondestructive analysis of inhomogeneous structures. Engineering and fabrication of new optical materials and structures for the research are performed in the technology group, using the pulsed laser deposition technique. A further area of research is focused on development of a dynamic theory of X-ray diffraction on perfect crystals and the utilization of results for the design and realization of new X-ray optical elements based on Si and Ge single crystals. In this area we are able to realize many novel X-ray monochromator elements and test them at European synchrotron facilities in collaboration with the X-ray optics groups of these facilities. The next important research area in the department is biophysics. This research is mainly focused on interactions of living objects with non-thermal plasma and high gradient magnetic fields.

### Research Highlights

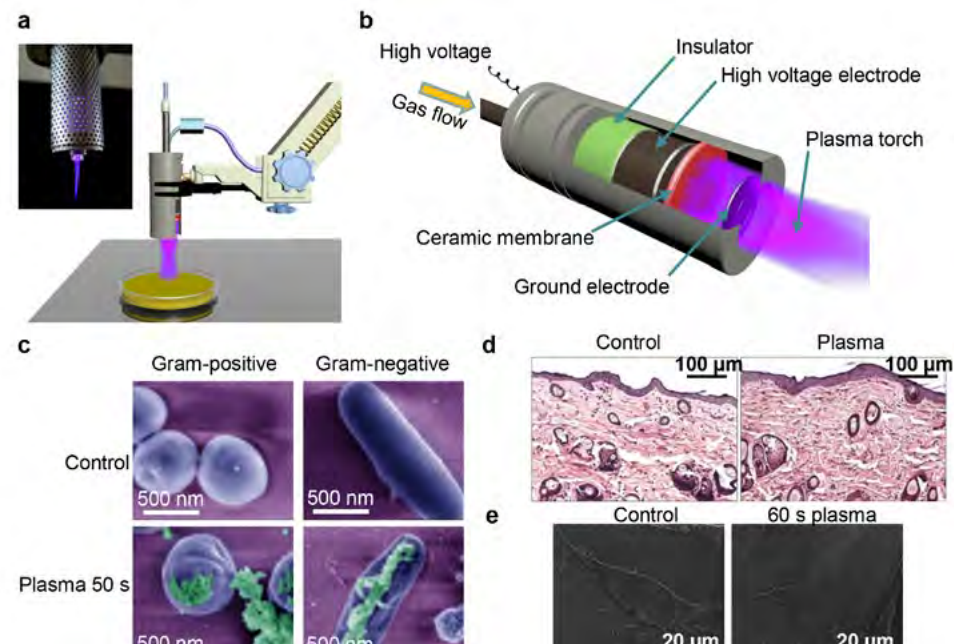
#### Biophysical Studies at the Frontier of Cell Biology

Biophysics represents an interdisciplinary science that encompasses methods and theories from physics to study biological systems. Its scope spans all levels of biological organization (from single molecules to whole organisms and ecosystems). A remarkable increase of interest in advanced biophysical methods for the investigation of structure-function relationships in proteins, organelles and cells has emerged in recent years. Moreover, new biophysical research directions having huge application potential in biology and medicine have appeared, such as: effects of high-gradient magnetic fields on living cell machinery, magnetically controlled stem cell delivery and plasma medicine. These research directions are actively studied in the department.

In recent studies, we demonstrated that plasma treatment completely destroyed both Gram-positive and Gram-negative bacteria within one minute of exposure (Fig.1) [1]. We showed that depending on the exposure time plasma induces either

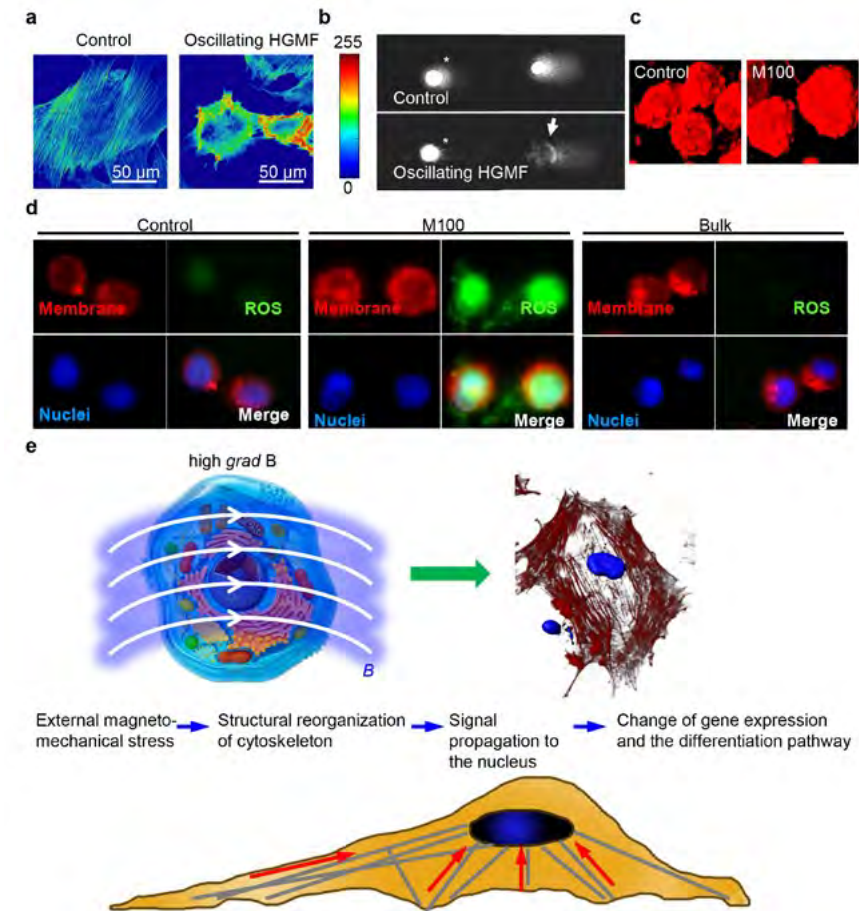
direct physical destruction of bacteria or triggers programmed cell death that exhibits characteristic features of apoptosis. The interaction of plasma with mammalian cell cultures (3T3 fibroblasts) induced cell death via the formation of multiple intracellular reactive oxygen/nitrogen species [2]. Our results showed a discrepancy in the superoxide accumulation and lysosomal activity in response to air and helium plasma, suggesting that the triggered signaling cascades might be grossly different between different plasmas. In addition, the effects of ozone, a major component of non-thermal plasma, have been simultaneously evaluated and have revealed much faster and higher cytotoxic effects [2]. On the other hand, when tested on intact rat skin, histopathological analysis did not reveal any harmful effects on plasma-treated animals in comparison to control ones [1]. Repeated plasma-treatment (1 or 2 min) of an open skin wound model for 3 days modulated expression of inflammatory markers. Our findings offer a novel insight into plasma-induced cellular responses, and provide a basis for the development of new methods of therapy.

The group is also conducting extensive research into the biological effects of high-gradient magnetic fields. Considerable effort has been expended to answer fundamental questions in Cell Biology, for instance: What happens when a living cell



**Fig. 1:** (a) Scheme of plasma system and image of the plasma torch. (b) Schematic diagram of plasma nozzle. (c) False-coloured SEM images of bacteria exposed to plasma. (d) Histopathological analysis of hematoxylin-eosin-stained rat skin sections from untreated (control) and plasma treated rats. (e) Scanning electron micro-photographs of untreated (control) and plasma treated mesenchymal stem cells.

interacts with a strong magnet of similar size to itself? How will a cell respond and adapt itself to a high magnetic field gradient? Many big questions remain to be answered before we reach understanding of cellular mechanics. As a significant contribution to this, we revealed the dramatic impact of a high-gradient magnetic field on the spatial organization and growth of stem cells [3].



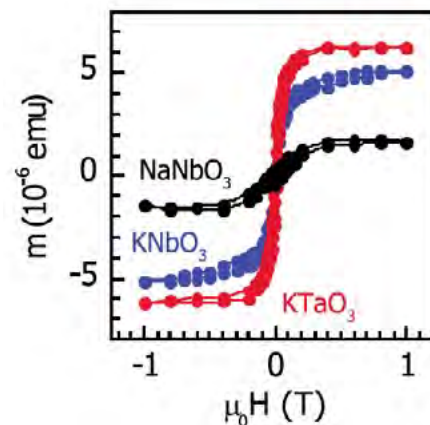
**Fig. 2:** (a) Stem cells were exposed to either mechanical vibrations or an oscillating HGMF for 7 days. After the treatment cells were fixed and stained for F-actin filaments. The fluorescence distribution and intensity of F-actin are shown in the reported pseudo-colour scale. (b) Detection of changes in DNA organization upon oscillating HGMF exposure for 5 days. Nucleoids with low (asterisk) and high level of DNA damage; arrows show disorganized structure of intact DNA. (c) Prolonged exposure to static high-gradient magnetic fields induces swelling of monocytic THP-1 cells. (d) Prolonged exposure to static high-gradient magnetic fields induces formation of reactive oxygen species (ROS). (e) Scheme of HGMF action on subcellular level.



In particular, we demonstrate that exploiting high-gradient micro-magnet arrays can induce swelling and apoptosis of human leukemia THP-1 cells as well as inhibit cell proliferation in the absence of chemical or biological agents. Under a prolonged exposure to a high-gradient magnetic field THP-1 cells were observed to swell up to 90 % in volume (Fig. 2) [4]. Mechanical stress, rising due to the magnetic gradient forces exerted on a cell, is shown to be responsible for triggering of cell swelling, formation of reactive oxygen species followed by apoptosis [4]. Furthermore, we showed that oscillating high-gradient magnetic field (HGMF) and mechanical vibration affect adipogenic differentiation of mesenchymal stem cells by the transmission of mechanical stress to the cell cytoskeleton, resulting in F-actin remodeling and subsequent down-regulation of adipogenic genes [5]. Our results showed that low-frequency oscillating HGMF and mechanical vibration reduced the adipogenic differentiation of MSCs. Furthermore, the presented results imply that both oscillating HGMF and mechanical vibration may affect adipogenic differentiation by the applied mechanical stress channeled along cytoskeletal filaments. Indeed, forces acting on the nucleus might induce changes in its shape, modify higher-order DNA organization, and thereby alter gene transcription (Fig.2).

### Strain and Interface Effects in Epitaxial Perovskite Structures

Perovskite-type metal oxides exhibit a variety of electronic phases and ferroic orderings which make these materials multifunctional and enable numerous applications. Conceptually new devices can be created using advanced oxides, in which composition-dependent or epitaxy-controlled nanoscale phenomena lead to novel or improved response functions. One of the fundamental problems here is detection of the phase states in ultra-thin perovskite epitaxial films (a couple of nm thick). We succeeded in the analysis, revealing the phase states of such films using the temperature-dependent ellipsometric studies. For example, in this work [6] we demonstrated the existence of the predicted strain-induced ferroelectric ordering in quantum paraelectric  $\text{KTaO}_3$  epitaxial films by combining experimental study and density functional theory calculations. The proof of the existence of the ferroelectric state was obtained from ellipsometry experiments. One of the fundamental problems in this quest is the determination of electronic energies and

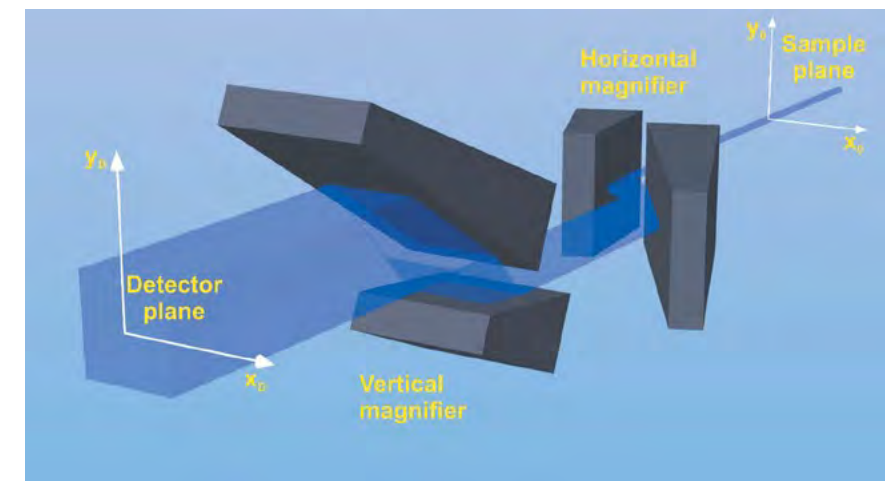


**Fig. 3:** Magnetization curves of as-deposited films of  $\text{KTaO}_3/\text{SrTiO}_3$  (red),  $\text{KNbO}_3/\text{SrTiO}_3$  (blue), and  $\text{NaNbO}_3/\text{SrTiO}_3$  (black) measured by SQUID at room temperature

excitations in these materials. Through combining optical ellipsometric studies, macroscopic examination of the order states, and materials characterization, we intend to explore connections between electronic transitions and ordering behavior that contribute to fundamental understanding of perovskite-type oxides and nanoscale phenomena therein. We recently found d0 ferromagnetism at a charge-imbalanced interface between two non-magnetic perovskites. Epitaxial  $d^0$   $\text{SrTiO}_3/\text{KTaO}_3$ ,  $\text{SrTiO}_3/\text{KNbO}_3$ , and  $\text{SrTiO}_3/\text{NaNbO}_3$  interfaces were observed experimentally by transmission electron microscopy and their optical properties were determined from spectroscopic ellipsometry measurements [7]. Magnetic measurements of these samples demonstrated ferromagnetic hysteresis at room temperature (Fig.3). Even though the observed phenomenon is mainly important for the basic research, its application potential is also very significant. Use of such interface-induced magnetism allows the development of new materials combining ferroelectric and ferromagnetic ordering (magnetoelectric multiferroics) without any magnetic elements.

### X-Ray Crystal Optics for Synchrotron Radiation

The main activity in this area is the research and development of new X-ray optical elements based on Si and Ge single crystals (Fig. 4). For example, it was recently shown that a cut in a certain direction in the X-ray monochromator can, after diffraction, cause the change of a polychromatic and parallel incident beam to one that is spatially spread with wavelength dispersion. This may be utilized for compression of properly chirped X-ray pulses [8]. The research of X-ray optical elements is carried out in a close cooperation with such local and international partners as the Czech company Polovodice a.s., Masaryk University in Brno, and Paul Scherrer Institute (Swiss Light Source) [9]. The



**Fig. 4:** Experimental setup for testing of the developed magnification system with special arrangement of Ge crystals.

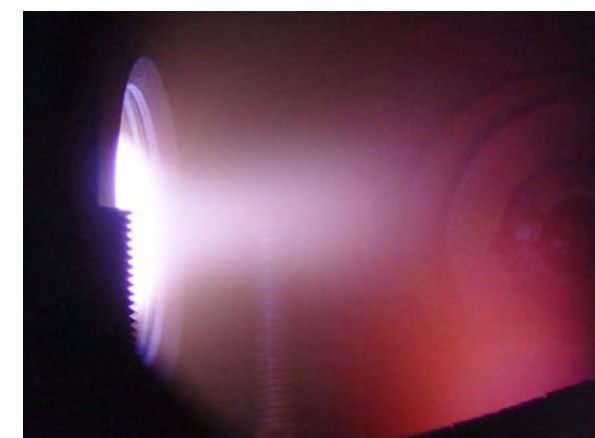
tests of some elements are performed at European synchrotron facilities wherein the elaborated methods are tested experimentally.

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## Department of Low-Temperature Plasma

The Department of Low-Temperature Plasma is focused on basic and applied research of new low temperature plasma sources employed for the deposition of and research on thin films and structures for various applications. These systems are suitable for the PVD (physical vapor deposition) and PECVD (plasma enhanced chemical vapor deposition) of thin film materials. The main scientific topic studied is the deposition of thin films and multilayer structures for photocatalysis and solar water splitting applications by the low temperature plasma systems. Mostly oxide materials based on  $\text{TiO}_2$ ,  $\text{Fe}_2\text{O}_3$ ,  $\text{WO}_3$  are investigated for these purposes. These films are prepared using a high power pulsed reactive magnetron and hollow cathode sputtering apparatus in various modifications and by a plasma chemical PECVD microwave surfatron multi-plasma jet system. These experimental facilities were developed and investigated in our department. The next important field studied is the advanced plasma diagnostics of depositing plasma. These studies help us to better understand and control deposition processes. Some of these measurements are done directly during the deposition "in situ". Several new time-resolved methods were developed for the diagnostics of pulsed depositing plasma, e. g., the system for time resolved laser absorption spectroscopy and the system for time-resolved probe plasma diagnostics of oscillating and unstable plasma. These methods are combined with the advanced newest commercial plasma diagnostics methods available in our department as for example time and energy resolved ion mass spectrometry and optical emission spectroscopy.



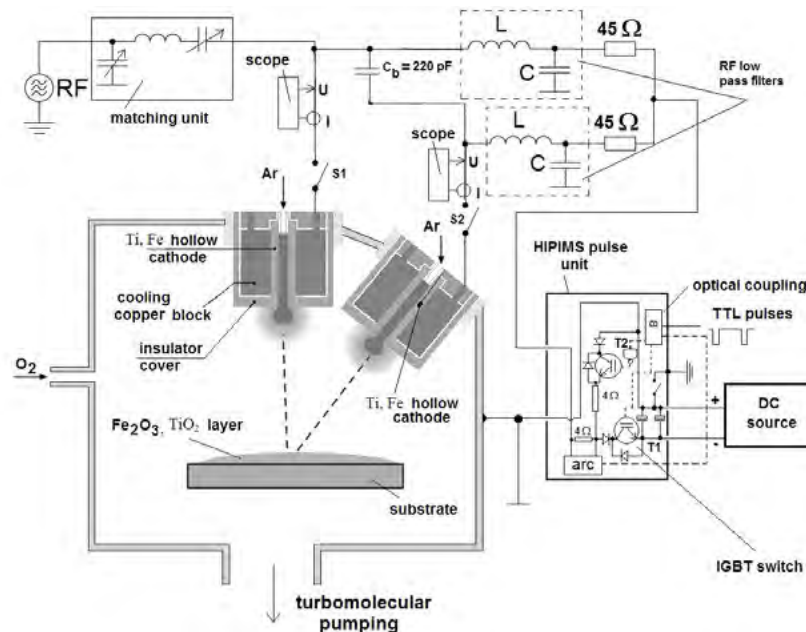
**Fig. 1:** Photography of high density high power pulsed magnetron plasma



## Research Highlights

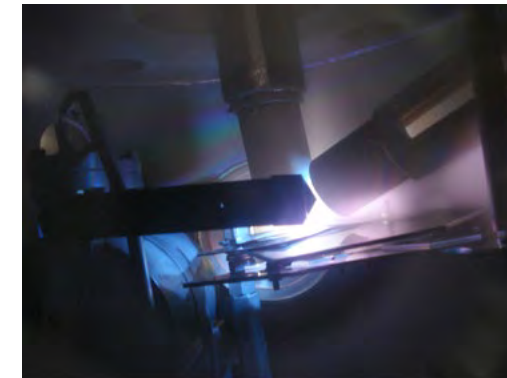
### Deposition of Thin Films for Photocatalytic and Solar Water Splitting

Since 2010 we have focused on the preparation of semiconducting materials for photocatalytic applications and solar water splitting by means of new low temperature pulsed plasma sources. The goal was to prepare these semiconducting materials with a high quality, defined microstructure and good photocatalytic properties. At first, we deposited  $\text{TiO}_2$  thin films with a crystalline phase of anatase or rutile on different



**Fig. 2:** Dual pulsed hollow cathode plasma jet system for reactive sputtering of oxide semiconductor thin films.

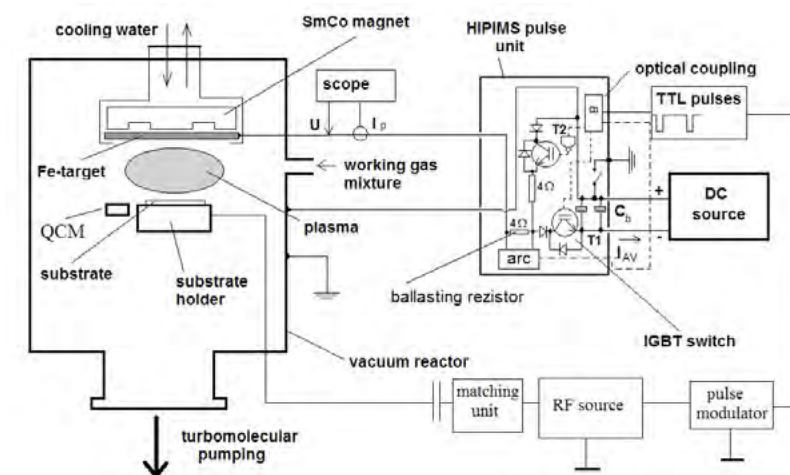
type of substrates. Further  $\text{Fe}_2\text{O}_3$  thin films with a hematite structure and  $\text{WO}_3$  films with a monoclinic phase were prepared using these low temperature plasma sources. These materials have lower band gap than  $\text{TiO}_2$  and consequently higher solar sensitivity. Our developed plasmatic methods were made it possible to also prepare these materials, in certain conditions, on thermally sensitive substrates. For this purpose, several low temperature plasma systems were developed. The pulse multi-plasma jet hollow cathode reactive sputtering system (see Fig. 1) was used for these depositions of  $\text{TiO}_2$  anatase and  $\text{Fe}_2\text{O}_3$  hematite. Materials of hollow cathodes (Fe, Ti) were sput-



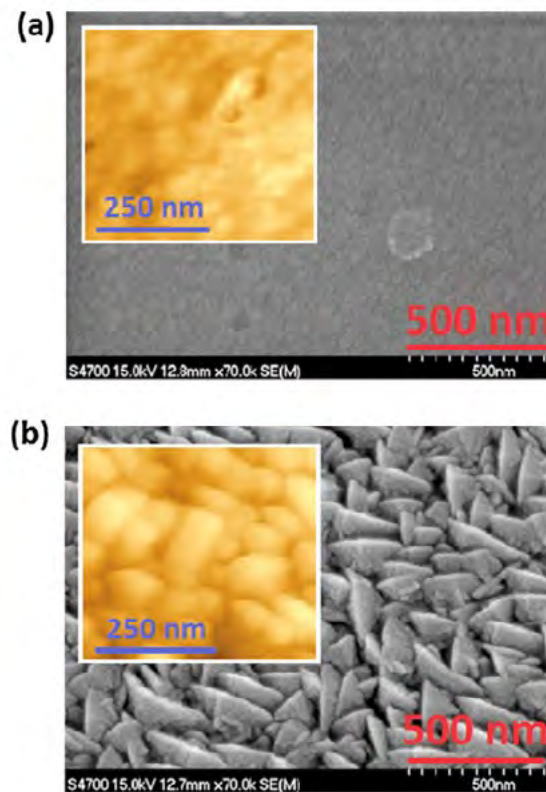
**Fig. 3:** Photography of dual hollow plasma jet system.

tered by a high density hollow cathode plasma and this material was carried by flowing plasma to the substrate (see Fig. 3).

A big advantage of this system is the very high deposition rate for reactive deposition of oxide films and simultaneously quite good semiconductor quality. We have deposited, using this system, high quality anatase  $\text{TiO}_2$  with relatively high photocurrents as shown by photoelectrochemical analysis. Similarly hematite  $\text{Fe}_2\text{O}_3$  semiconducting films prepared by this system were suitable for solar water splitting applications.



**Fig. 4:** Pulsed high power magnetron system for reactive sputtering of oxide semiconductor thin films.

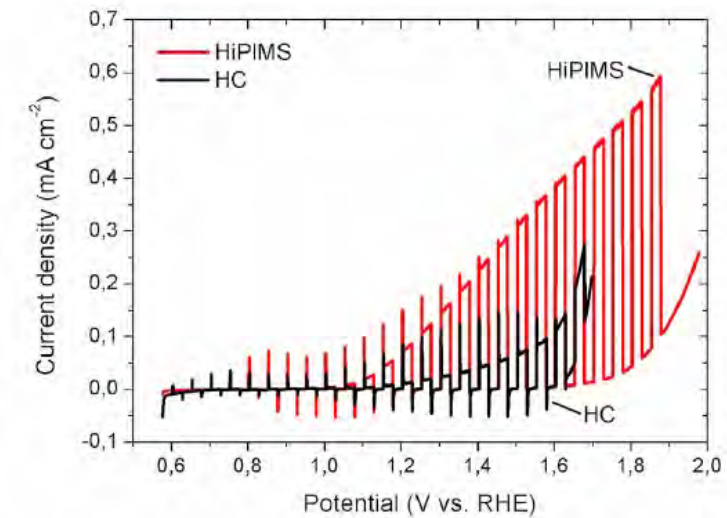


**Fig. 5:** Surface properties of hematite  $\text{Fe}_2\text{O}_3$  thin films deposited by pulsed hollow cathode (HC) and high power pulsed magnetron sputtering (HIPIMS).

A reactive high power pulsed magnetron sputtering system was applied for the deposition of semiconductor oxides. Hybrid combination of different pulsed plasma excitation frequencies allows us to control the structure, texture and photocatalytic semiconductor properties of these thin films

A significant increase in thin film quality was achieved by implementation of developed time resolved “in situ” plasma diagnostics of depositing particles. Energy and ion flux on the substrate are very important parameters effecting crystalline structure and texture of deposited films.

Developed “in situ” pulsed plasma diagnostic systems enabled us to become a consortium member of the FP7 research project HIPPOCAMP funded by the EC. Developed plasma deposition systems are the subject of the applied research of depositions of optical thin films within the framework of a TACR project, run in co-operation with the industrial company Meopta Prerov. Our basic research is funded by the Czech Science Foundation.



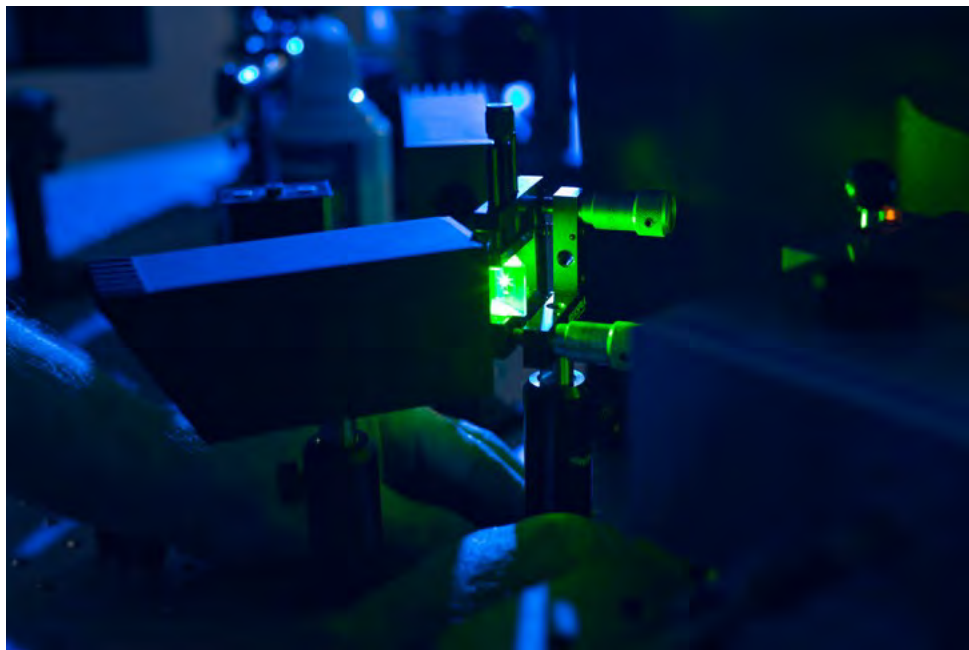
**Fig. 6:** Photoelectrochemical characteristics of hematite  $\text{Fe}_2\text{O}_3$  thin films at chopped light illumination with solar intensity 1 AM deposited by pulsed hollow cathode (HC) and high power pulsed magnetron sputtering (HIPIMS).



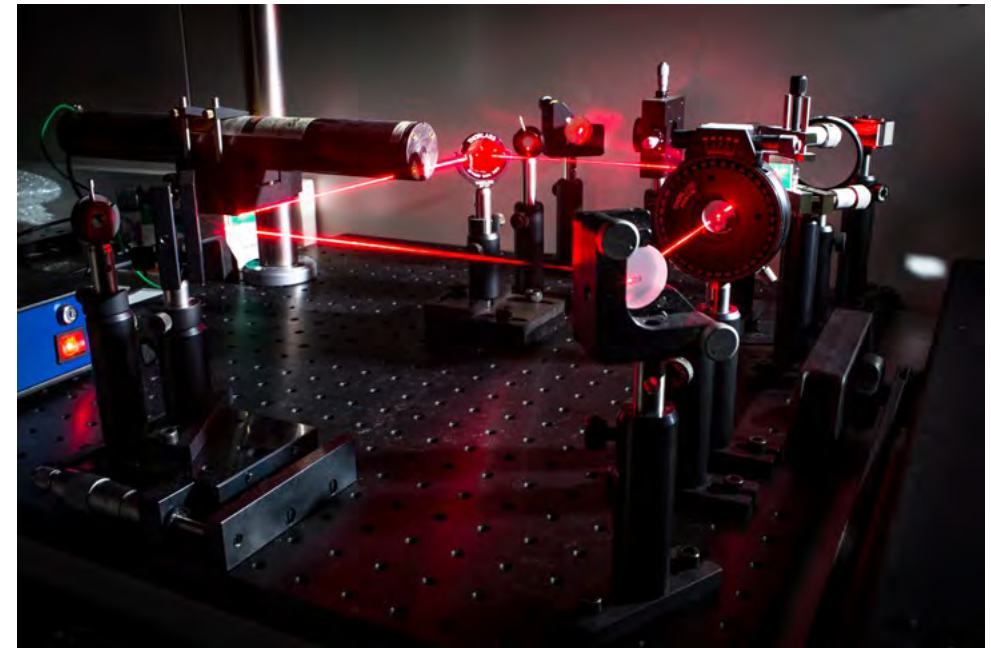
## Joint Laboratory of Optics

The Joint Laboratory of Optics is an institute jointly funded by the Institute of Physics and Palacký University. In the structure of the Institute of Physics it is a department of Optics Division, while in the structure of the University it is placed as a department of the Faculty of Science. Since 2010, the laboratory also serves as one of the research divisions of the Regional Centre of Advanced Technologies and Materials established at Palacký University.

The laboratory is focused on both fundamental and applied research in various areas of optics, particle physics and material science. It is divided to five scientific and three service groups. The group of quantum and nonlinear optics deals with quantum properties of light fields at the level of single photons, applicable to the areas of quantum information processing, quantum metrology, detection of photons and photon statistics. The group of applied optics is focused on the design and manufacture of specialized optical components that find their application in the industry or in large scientific collaborations (e.g., the Pierre Auger Collaboration). Related technologies



**Fig. 1:** Detail of an optical setup for quantum information processing



**Fig. 2:** Interferometric setup used for single-photon experiments

of production and quality-control of surfaces and layers using large diameter grinding and polishing, vacuum streaming and plasma deposition are also developed. The group of wave optics deals with non-contact optical measurement methods based on speckle or white-light interferometry. The particle physics group contributes to the CERN-ATLAS experiment mainly in the area of modeling of optical detection processes. The last of the scientific groups – the group of optoelectronics – develops microelectronics and optoelectronics systems for industrial partners of the laboratory. Three support groups – the optical workshop, the mechanical workshop, and an administration section – ensure the smooth running of the scientific groups.

## Research Highlights

### Quantum Information

Exploring the properties of the quantum microworld has led to the rise of a new area of scientific inquiry – that of quantum information. Quantum information processing enables faster computational algorithms to be implemented, as well as faster methods of searching databases and safer methods of communication than are achievable with the methods of classical physics. The quantum and nonlinear optics group studies

quantum algorithms and protocols with the aim of bringing the field closer to practical applications. In our laboratories individual photons are employed as carriers of quantum information and with the help of single- and two-photon interference, information processing takes place. Among the most significant results recently achieved in this area is the implementation of a tunable phase gate [1]. It is a prominent member of the family of elementary quantum-information tools. It may be used as a building block for a broad range of quantum information tasks. In addition, this implementation was the first to offer full tunability and the maximum efficiency permitted under the laws of quantum physics. Another laboratory result in this area is a multifunctional quantum cloning device, the analogue of a classic copier but controlled by the laws of quantum physics. It is capable of duplicating an unknown quantum state with the maximum level of precision allowed by quantum physics. Such a device may be used for efficient eavesdropping on quantum cryptography [2]. Experimental testing of the resistance of quantum cryptography contributes to determining the limits of its security.

In addition to the design and construction of elements for the quantum processing of information, the laboratory also focuses on the design of original detection schemes for analyzing the properties of two-photon states of light and designing new elements and structures for the generation of photon pairs. The group has designed new methods for analyzing the quantum state of paired fields applicable for absolute calibration of detectors at the level of individual photons [3]. These methods are



**Fig. 3:** Dr. Libor Nožka checking the surface of a deposited layer of the mirror manufactured at the Joint Laboratory of Optics for the Pierre Auger Observatory.

also capable of generating multiphoton nonclassical states of light [4] which are unparalleled in classical physics and are distinguished by lower noise levels than would be achievable within classical physics.

### All-Sky Cameras

A number of scientific and industrial facilities that do their work under the open sky are dependent upon the state of the atmosphere or the amount of precipitation and cloud cover. Long-term monitoring of the atmosphere at often remote locations targeted for the construction and future operation of such facilities is essential in selecting a location effectively. To ensure the functioning of a number of operations and facilities that require clear skies, the ability to monitor the level of cloudiness both day and night is crucial.

All-sky cameras developed in the laboratory are a by-product of involvement in large international scientific collaboration projects. Currently, they are in use as part of two projects – at the Pierre Auger Observatory (in Argentina, four camera systems installed) and at the Cherenkov Telescope Array (a total of seven systems installed in Namibia, Mexico, USA and the Canary Islands). A reference system has been also installed near Olomouc. These are autonomous cameras, highly flexible and capable of many different uses. They are capable of monitoring the intensity of light of the night sky background with an angular resolution of about  $1.5^\circ$ . They can also be used for long-term monitoring of day and night cloud coverage levels and the brightness of the night sky. This is highly useful, for example, in planning the location of future observatories, registering the effects of light pollution near urban agglomerations and increasing the efficiency of operation of systems and facilities that are dependent upon a clear sky.

Besides the cameras, the laboratory contributed to the Pierre Auger Observatory by supplying to it the unique mirrors with extremely low scattering that constitute a fundamental building-block of the fluorescence telescopes of the observatory.

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A photograph of two scientists in white protective suits and goggles working on a complex mechanical device in a laboratory. The device has various pipes, valves, and a blue light source. The background shows a laboratory setting with shelves and equipment.

Institute of Physics  
The Czech Academy  
of Sciences

Division of High  
Power Systems

The origins of the division date back about 35 years. At that time, the institute decided to establish a new laser laboratory equipped with a 100 GW iodine laser facility, known as PERUN, which was used for the research of laser driven X-ray and ion sources. The PERUN facility was constructed in cooperation with the Lebedev Institute of Physics in Moscow. A successful operation of the PERUN facility and a re-orientation of the research programme at MPQ Garching supported efforts for the ratification of the Euratom-assented agreement on the transfer of the iodine laser system Asterix IV between the MPQ and the Czech Academy of Sciences. At the end of 1998, Asterix IV was transferred to the new research centre Prague Asterix Laser System (PALS), which was established as a joint laboratory of the Institute of Plasma Physics and our institute to exploit this powerful tool. The PALS facility has been serving the worldwide research community since September 2000.

A world leading successful experiment was carried out at the PALS facility by the team of researchers from our division in the field of collisionally excited, highly coherent XUV laser at 21 nm. Other unique experiments were devoted to the formation of plasma jets and generation of highly ionized heavy elements. The outstanding results obtained at the PALS facility influenced the decision of the Steering Committee of the ELI consortium, made in September 2010 to give a mandate to the Czech Republic to implement the ELI Beamlines facility as one of three facilities of the future European ELI-ERIC Infrastructure in Dolní Břežany. Due to the very fast increase of the number of employees working in ELI Beamlines research, technology and administration, a new ELI Beamlines Project Division of the institute was created on April 1, 2012. Since then, the newly re-organized Division of High Power Systems is composed of two scientific departments and one department of technical support. The first Department, of Radiation and Chemical Physics, mostly deals with high peak power phenomena and high energy density physics while the second, the Department of Diode-Pumped Lasers, is focused on strategic research and the development of high average power lasers for real-world applications.

The Division consists of two departments:

- Department of Radiation and Chemical Physics **p. 197**
- Department of Diode-Pumped Lasers **p. 206**

## Department of Radiation and Chemical Physics

Research activities of the department are located at the frontier of high-energy-density physics and high-energy chemistry. The research streams are elaborated below: (1) interaction of intense extreme ultraviolet and soft X-ray radiation with matter of various kinds, from elemental solids to biomolecular systems, (2) X-ray, extreme ultraviolet and optical emission spectroscopy of plasmas produced by focused beams of short-wavelength and conventional, long-wavelength lasers, (3) characterization and application of neutrons and charged particles emitted under these interaction conditions, (4) other advanced diagnostic techniques, including imaging and pump-and-probe, utilized in the study of laser-produced plasmas, (5) characterization and application of focused beams of short-wavelength lasers, (6) X-ray holography with atomic resolution and related techniques, (7) chemical and plasma-chemical generators of atomic and excited species for chemical lasers and related purposes, (8) chemical consequences of laser-induced dielectric breakdown in molecular gases and their mixtures, and (9) theory and computer simulations of hot dense plasmas and warm dense matter. In the above-mentioned areas, both fundamental and application-motivated research is conducted at large-scale facilities operating abroad (FLASH in Hamburg, LCLS at SLAC in Menlo Park – CA, LULI in Palaiseau, CELIA in Bordeaux, SCSS and SACLA in Japan, ELETTRA in Trieste, and many others) as well as at the Institute using the PALS facility (a kJ-class iodine photo-dissociation laser system providing sub-nanosecond pulses of near-IR radiation; PALS – Prague Asterix Laser System). The motivation comes mostly from inertial confined fusion research and technology, laboratory astrophysics and astrophysics, materials science and processing, radiation chemistry and biophysics, etc.

### Research Highlights

#### Interaction of Intense Short-Wavelength Radiation with Matter

Interaction of extreme-ultraviolet radiation (XUV;  $10 \text{ nm} < \lambda < 100 \text{ nm}$ ) and soft X-rays (SXR;  $0.2 \text{ nm} < \lambda < 30 \text{ nm}$ ) with matter differs dramatically from that of long-wavelength (i.e., UV-Vis-IR) radiation. The interaction of short-wavelength radiation with matter occurs mostly due to the photo-effect in atoms of the irradiated material. Valence electrons play a minor role in the interaction in general. Thus an absorption coefficient depends on the elemental composition and density of the irradiated material. Contrary to long-wavelength radiation, there is a little influence of the fine chemical structure of the particular material chosen for an irradiation.

In addition to this, short-wavelength radiation is deposited much more effectively in the material because the effect of plasma reflection of laser light is reduced. It follows



from the fact that in a certain spatial position in the plasma, where the oscillation frequency of plasma electrons (so called plasma frequency and/or Langmuir frequency) oscillating in the electromagnetic field is equal to the frequency of laser radiation, the index of refraction becomes zero and the electromagnetic wave is reflected. Langmuir frequency is a function of electron density ( $n_e$ )

$$\omega_e^2 = n_e e^2 / \epsilon_0 m_e$$

Laser frequency is equal to the Langmuir frequency at the critical density which depends on the laser wavelength in the following way:

$$n_c \text{ [electrons in cm}^3\text{]} = 10^{21} \times \lambda^{-2} \text{ [\mu m]}.$$

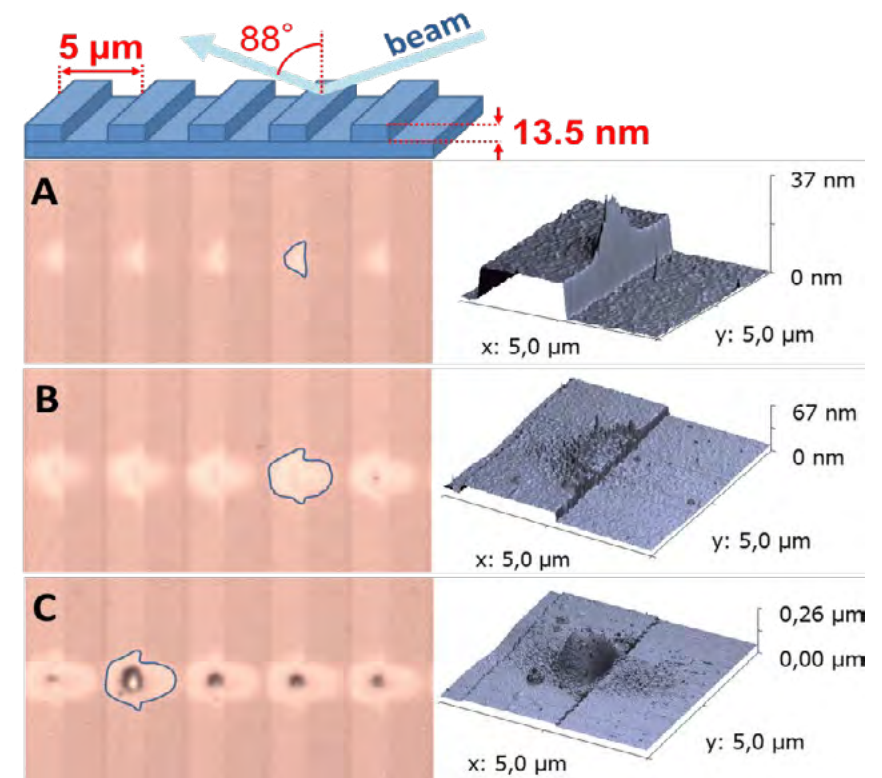
Let us compare a typical XUV and VUV laser from this point of view. A critical density  $n_c = 5 \times 10^{23} \text{ cm}^{-3}$  can be expected for 46.9-nm radiation in the XUV spectral range. This means that the XUV-laser radiation can penetrate all the parts of the plasma formation volume with an electron density  $< 5 \times 10^{23} \text{ cm}^{-3}$ . This value is comparable to an electron density of solids. Therefore the sample can be heated by the short-wavelength radiation in the whole volume irradiated. Hence the technique is called volumetric heating. In comparison, the critical density is at least 15x smaller for an ArF excimer laser. An expanding ArF-laser-induced plasma plume begins to reflect the 193-nm laser radiation at a certain moment of the interaction course. Therefore the volumetric heating of solids cannot be carried out with VUV (and of course UV-Vis-NIR-IR) laser radiation.

### X-Ray Lasers Produce Unique Plasmas

An international team of researchers created a unique state of matter due to the above-mentioned volumetric heating of aluminium induced by a tightly focused beam of X-ray free-electron laser LCLS (Linac Coherent Light Source) in California. Solid-density plasmas at a temperature exceeding  $10^6 \text{ K}$  were produced under these irradiation conditions [1].

Matter with a high energy density ( $> 10^5 \text{ J/cm}^3$ ) is prevalent throughout the universe, being present in all types of stars and towards the centre of the giant planets; it is also relevant for inertial confinement fusion (ICF). Its thermodynamic and transport properties are challenging to measure, requiring the creation of sufficiently long-lived samples at homogeneous temperatures and densities. An understanding of the contrasting case of intense X-ray interaction with dense systems is important from a fundamental viewpoint and for applications.

Detailed simulations of the interaction process conducted with a radiative-collisional code showed good qualitative agreement with the experimental results. Insights into the evolution of the charge state distribution of the system, the electron density and temperature, and the timescales of collisional processes were obtained. The unique, but well-determined conditions were utilized for a systematic treatment of various



**Fig. 1:** Reflection grating (i.e., a structured silicon substrate covered by a 45 nm thick layer of amorphous carbon; a grating profile and irradiation conditions are displayed at the top of the figure) irradiated by a single shot of SXR FEL radiation at a fluence of (A) 356 mJ/cm<sup>2</sup>, (B) 806 mJ/cm<sup>2</sup>, and (C) 1115 mJ/cm<sup>2</sup> [10].

particular phenomena occurring in the dense plasmas [2–4]. Presented results should inform future high-intensity X-ray experiments involving dense samples, such as X-ray diffractive imaging of biological systems, material science investigations, and the study of matter in extreme conditions with motivation coming mostly from ICF, Earth, and Space sciences.

### Characterizing “Strange” Beams of XUV/X-ray Lasers

In the physics of extreme states of matter, it is important not only to approach an appropriate high-energy-density level but also to diagnose and characterize the system investigated under unsteady conditions. Therefore systematic experimental and the-

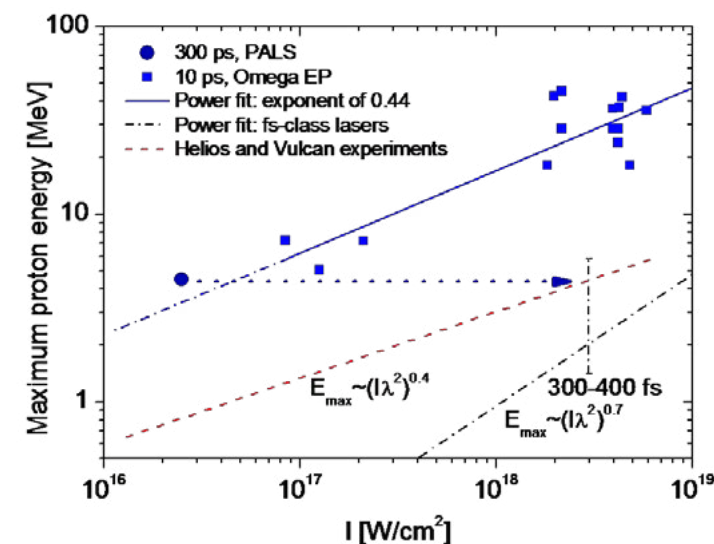
oretical works dealing with an accurate and reliable characterization of focused laser beams are conducted in our division to carry out the short-wavelength laser-matter interaction research properly. The detailed knowledge of transverse energy distribution within the beam profile turns out to be essential for interpretation of the quite nontrivial experimental results obtained at an enormous irradiance. Non-Gaussian beams, which are typical of XUV/SXR-ray lasers, require rigorous study as well as the interactions induced by them. Our recent work is therefore devoted to a detailed characterization of focused general laser beams [5, 6] extending the ablative imprint technique published earlier [7].

### Are Diamonds Really Forever?

It follows from the above paragraphs that high-performance optics is needed to concentrate energy of the XUV/X-ray laser beam on solid targets to produce dense plasmas. Of course, an optical element itself is heavily exposed to short-wavelength laser radiation. Any element of the beam guiding and focusing system should be constructed, manufactured and operated under conditions which avoid damage by laser pulses. We are systematically studying responses of a wide variety of XUV/SXR optical materials to intense short-wavelength radiation. Our division organized a series of international conferences in this area. Proceedings of the fourth conference in the series appeared in 2013 [8].

A typical element often considered for fabricating the optics is carbon. We have already investigated several allotropes of this light element, i.e., diamond, graphite, amorphous carbon, and fullerenes. For example, diamond samples were irradiated by free-electron laser femtosecond pulses at XUV/SXR photon energies ranging from 24 to 275 eV [9]. Micro-Raman analysis evidenced the graphitization of the irradiated diamond samples. The fluence threshold for graphitization was retrieved for all radiation photon energies using Nomarski (differential interference contrast) microscopy. A dedicated theoretical approach was applied to model the short wavelength laser-matter interaction. Comparison of the experimental and theoretical values shows their good agreement, indicating the non-thermal nature of the graphitization process initiated by intense extreme ultraviolet and soft X-ray radiation.

Not only a particular material of the substrate and coatings, but also spatial structure (i.e., single coating of different thicknesses, multilayer mirrors, grating-like structures, etc.) influences radiation resistance of optical elements. We studied an interaction of free-electron laser pulses with a grating structure using 4.6-nm radiation generated at the FLASH facility in Hamburg. For fluences above  $63.7 \pm 8.7$  mJ/cm<sup>2</sup>, the interaction triggers a damage process starting at the edge of the grating structure as evidenced by Nomarski optical and atomic force microscopy (Fig. 1). Simulations based on solution of the Helmholtz equation demonstrate an enhancement of the electric field intensity distribution at the edge of the grating structure. The ratio of the maximum energy absorbed in the grating to the energy absorbed on the surface of a flat mirror is found to be  $\gamma = 3.4$ . This value is directly related to the ratio of damage



**Fig. 2:** Proton scaling as a function of laser intensity: circle – protons from the rear surface of a 17- $\mu\text{m}$  Si target exposed to the PALS laser, squares – experiment performed with the 10-ps Omega EP [17]; dash line – experiment performed with the Helios and Vulcan lasers; dash dot line – experiments performed with fs lasers. The error bar corresponds to protons accelerated with 300–400 fs lasers.

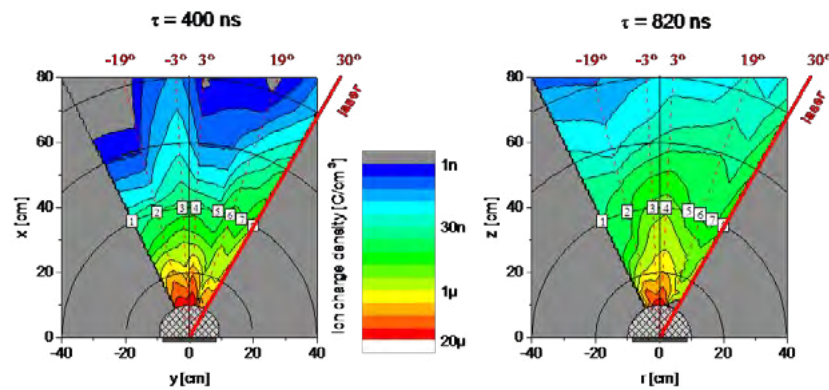
thresholds of the mirror and the grating determined in our irradiation experiment carried out at the FLASH facility.

### Ion Acceleration at the PALS Facility

Since the first studies of laser interaction with solid targets, the efficient emission of energetic ions from laser-generated plasmas has been of special interest for ion sources, especially for radiobiology, high quality collimated ion beams for nuclear reactions and radiation therapy as well as for material modification [11–15]. Although the conversion efficiency of the laser intensity into the ion kinetic energy decreases with increasing laser pulse duration [16], as Fig. 2 shows, the number of energetic ions generated with the use of the PALS facility delivering 0.3-ns pulses is very high. This fact allows, for example, us to produce a high yield of alpha particles of  $\sim 10^9$  per steradian from a well-defined layer of boron dopants in a hydrogen-enriched silicon target irradiated by the PALS laser with a nominal intensity of  $3 \times 10^{16}$  W·cm<sup>-2</sup> triggering the proton–boron nuclear reaction:  ${}_{11}\text{B} + \text{p} \rightarrow 3\alpha + 8.7$  MeV [17].

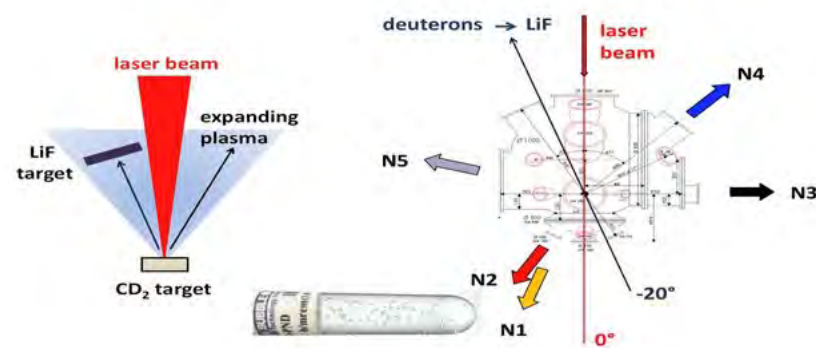
Optical energy of nanosecond laser pulses is not directly converted into the collective macroscopic motion of particles but also results into thermal effects causing instabilities and inefficiencies for macroscopic motion. With the aim of obtaining infor-





**Fig. 3:** Charge density maps of protons and carbon ions at the time of 400 ns and 820 ns after the interaction of a PALS-laser beam with a  $(CH_2)_n$  target. The labels indicate the directions of observation of ion currents with the use of eight ion collectors positioned at the distance of 40 cm from the target. The laser beam struck the target at the angle of  $30^\circ$ ; target irradiation of  $3 \times 10^{16} \text{ W/cm}^2$ .

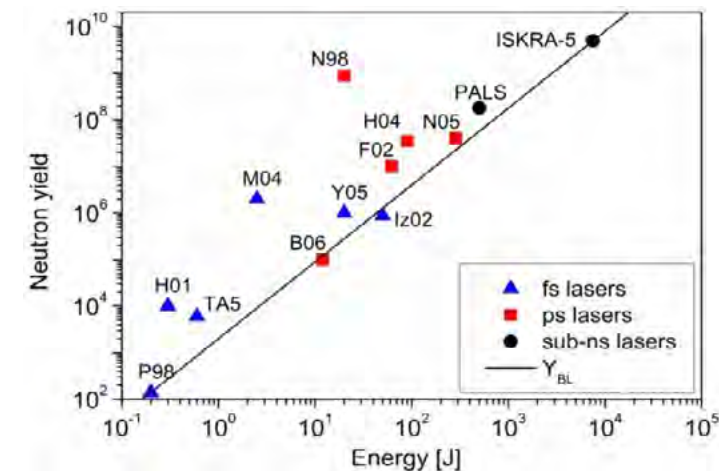
Information on the space distribution of the expanding plasma, we developed a new method of transformation of the time-resolved ion currents  $j(t)$  into the distance-of-flight (DOF) charge density profiles  $q(x)$  where  $x$  is the flight distance [18]. A set of the density profiles allows us to draw a map of ion charge density at a selected time  $\tau$  after the end of the laser pulse, as Fig. 3 shows.



**Fig. 4:** Left: diagram of the dual target configuration. Right: configuration of scintillation detectors N1 to N5 around the target chamber. Bottom: calibrated bubble dosimeter (BD-PND: The Bubble Detector – Personal Neutron Dosimeter) used for measurement of the dose of neutrons.

If a single planar deuterated polyethylene target is irradiated with the PALS laser, then accelerated deuterons are capable of initiating the  ${}^7\text{Li}(d,n){}^8\text{Be}$  reaction in a secondary LiF (catcher) target as well as the  $\text{D}(d,n){}^3\text{He}$ , and  ${}^{12}\text{C}(d,n){}^{13}\text{N}$  reactions in the primary target [19, 20]. The observed yield of neutrons from the  $\text{D}+\text{D} \rightarrow {}^3\text{He} + n$  (0.82 MeV) + n (2.45 MeV) nuclear reaction was of  $2 \times 10^8$  neutrons per laser shot for the average laser energy of 550 J [19]. Figure 5 shows a spread in the neutron yield dependence on the energy delivered on deuterated targets with the use of various fs-, ps- and sub-ns lasers. The spread can be limited by a baseline which was estimated to be  $Y_{BL} = 2000 \times E^{1.65}$ .

Deuterons with energies up to  $\sim 2.5$  MeV were accelerated from the front surface of a massive  $\text{CD}_2$  target in the backward direction with respect to the laser beam and impacted a 1 mm thick natural LiF slab, see Fig. 4. Neutrons emitted to all directions had a mean energy of  $\sim 13.5$  MeV. Only a minority of them reached up to  $\sim 16$ -MeV energy. The maximum neutron yield from both the primary and secondary reactions was  $3.5 \times 10^8$  neutrons per shot.



**Fig. 5:** Neutron yield per laser shot versus laser energy. Data from: P98 – Pretzler et al., 1998; H01 – Hilscher et al., 2001; TA5 – Ter Avetysian et al. 2005; M04 – Madison et al., 2004; Y05 – Youseff et al., 2005; Iz02 – Izumi et al., 2002; B06 – Belyaev et al., 2006; F02 – Fritzler et al., 2002; N05 – Norreys et al., 2005; N98 – Norreys et al., 1998; H04 – Habara et al., 2004; PALS – presented experiment; ISKRA-5 – Bessarab et al. 1992, see [19].

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## Department of Diode-Pumped Lasers

The department operates a new research and development Centre HiLASE which deals with the technological development of high average power pulsed lasers. HiLASE's "next generation" technology is based on diode pumped, solid state laser architecture that incorporates highly efficient laser emitting diodes to generate the intense light pulses that drive the laser amplifiers. This technology combines a unique combination of high average power, high pulse repetition rate and high efficiency. The main applications of these lasers include laser induced damage threshold measurement of optical materials, laser shock peening, development of compact extreme ultraviolet sources for lithography, mid-infrared generation, and laser micromachining. The activities of HiLASE are being developed in close collaboration with industrial users, universities and other research institutions worldwide. There are three research groups established within the HiLASE Centre: (1) development of pulsed kW class thin-disk diode pumped solid state laser systems with energy up to J-level for industrial and scientific applications, (2) development of a 100 J/10 Hz class multi-slab laser system and validation of computer codes to demonstrate scalability up to kJ level, and (3) development of future industrial applications of lasers in programmes 1 and 2, and advancement of key technologies for high repetition-rate amplifiers in partnership with industry. The Department of Diode-Pumped Lasers is a successor of the former Department of Laser Interactions which was disbanded in early 2014.

### Research Highlights

#### Power Scalability of PALS

Some basic research of laser-matter interactions requires very high intensity lasers. It is generally understood that every large laser consists of a very stable oscillator and many amplifiers to increase the output power and energy. However, the relationship is not linear and adding larger amplifiers has fundamental limitations. One of the reasons is that above a certain level the high intensity of the laser beam will destroy the lasing medium. However, a high output power laser beam can be achieved not only by harnessing energy, but also by shortening its pulse length. This brilliant idea is called *Chirped Pulse Amplification* (CPA) [1], it profits from the physical regularity that a short pulse has over a large frequency spectrum. However, the CPA method can be applied only to lasers with broad spectral bandwidth. An important question was: is there a possibility to increase the output power of lasers with a narrow spectral bandwidth, such as the iodine photodissociation laser system PALS? The answer is, yes, but the CPA method has to be modified to a *Optical Parametric Chirped Pulse Amplification*

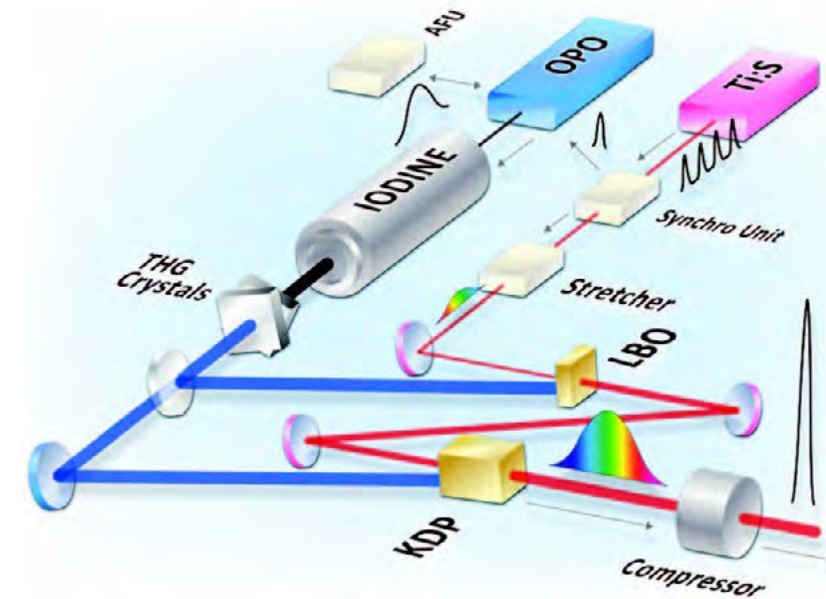
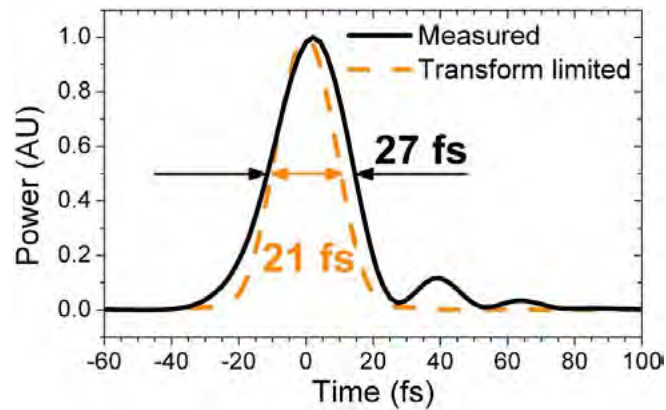


Fig. 1: Schematic of the OPCPA facility in SOFIA laboratory.

(OPCPA) method, another brilliant technique, invented in 1992 [2]. For OPCPA, two lasers are necessary. One is energetic (*pump*) with a narrow spectrum (e.g. a bandwidth of 20 picometers in the case of PALS), while the other laser (*signal*) has a very low output and very short pulse (i.e. possessing a broad spectral bandwidth), e.g. a Ti:sapphire laser (70 nm bandwidth). First, the Ti:sapphire beam is chirped in a stretcher, then a crystal with high optical nonlinearity is inserted in the beam path, and a synchronized energetic pulse is also injected. In the crystal, the energy of the latter pulse is transferred to the chirped Ti:sapphire laser pulse via the *optical parametric amplification* (OPA) process. After that the Ti:sapphire pulse is both energetic as well as spectrally broad. It was demonstrated [3, 4] that using this method the output power of the PALS laser beam would increase by three orders of magnitude!

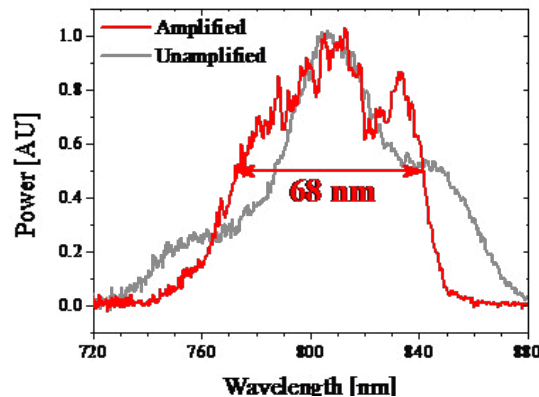
However, testing and implementation of the OPCPA technique at PALS would close this user facility for a long time. Therefore we built a small-scale iodine laser SOFIA (*Solid-state Oscillator Followed by Iodine Amplifiers*) for a pilot investigation of the applicability of the OPCPA technique for iodine laser [5], and later on for elaboration of a reliable design of the OPCPA upgrade for the PALS system. The SOFIA beam was frequency tripled and pumped a two-stage OPA consisting of one LBO and one KDP crystal, as shown in Fig. 1. The fs signal beam from a Ti:sapphire laser was chirped in a home-made stretcher consisting of a single gold-coated diffraction grating and an Öffner telescope [6, 7]; the pulse duration increased from 12.5 fs to 250 ps. Note that the success of this OPCPA system was achieved thanks to an advanced synchronization

**Fig. 2:** Temporal evolution of the TW pulse (solid black) compared with its theoretically possible pulse shape (dashed orange).



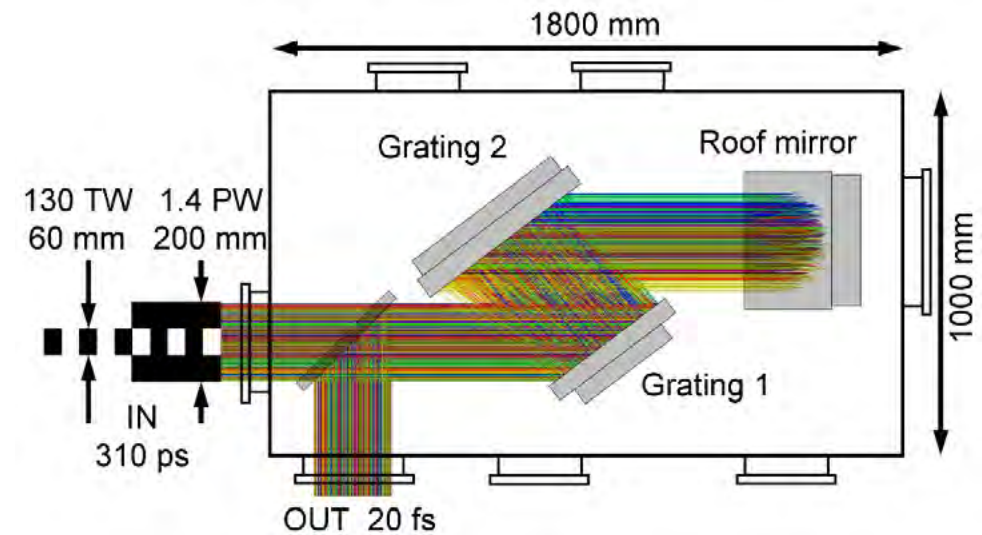
of three laser systems running at different repetition rates: 75 MHz (Ti:sapphire laser), 10 Hz (solid-state oscillator of the SOFIA system), and single-shot (iodine amplifiers). By the way, matching the narrow line of the solid-state oscillator to the narrow line of the iodine amplifiers ( $1315.24 \pm 0.02$  nm) was another hard nut to solve. This was the first time that a single-shot ( $1 \times$  per 10 min) two-stage OPA was driven by a very narrowband gas pump laser, and also the first time that an fs pulse at 800 nm was amplified in a KDP crystal [8], as shown in Fig. 2. The signal was amplified over 108 times (!) and after compression, the output power was 1.5 TW and the pulse duration was 27 fs. The largest amplified spectral bandwidth was 68 nm which corresponds theoretically to the shortest-possible pulse duration of 14 fs [9], as shown in Fig. 3. We further studied the stability conditions of the OPCPA amplifiers under mismatching of the angles and arrival of the signal and pump beams into the nonlinear crystals [10].

The numerical and experimental results obtained on the small-scale SOFIA system provided a good basis for our design of a petawatt OPCPA upgrade of the kJ iodine laser PALS [11]. The design aimed at the generation of two ultra-high power laser beams, 130 TW and 1.4 PW, which would be formed in a chain of several OPCPA



**Fig. 3:** Spectrum of a  $10^8$  times amplified pulse of maximal bandwidth compared with the seed spectrum.

amplifiers. The front-end of the chain is based on three BBO crystals pumped by a frequency doubled Nd:YAG laser at a repetition frequency of 10 Hz. Two KDP crystals are pumped by the frequency tripled PALS beam (i.e. at a single shot repetition rate). If only one KDP crystal is used, the 130 TW beam is available for target experiments. An optional 1.4 PW beam is produced if the beam leaving the first KDP crystal is further amplified in the second KDP. The energy of the outgoing beam is 34 J. The subsequent optical compressor (Fig. 4) can temporally compress the beam down to 27 fs. Using the OPCPA scheme the output power of the PALS laser system would be increased by three orders of magnitude! Thus a reliable design for the possible OPCPA upgrade of the PALS laser system has been completed [11]. However, in the meantime another two large scale laser projects, based on the very progressive technology of diode pumping, have been approved: ELI (*Extreme Light Infrastructure*) and HiLASE (*High*



**Fig. 4:** Top view of the signal beam ray tracing through the grating compressor for both the 130 TW and 1.4 PW top-hat beams of 60 mm and 200 mm diameters, respectively, inside the proposed compressor chamber [4].

average power pulsed LASERs). Therefore, the proposed design for petawatt upgrade of the PALS laser system will not be finally realized.

Besides the OPCPA research we also focused on ultrashort laser pulse diagnostics. A new, highly simplified technique for ultrashort pulse measurement and retrieval was developed. The technique, which is analogous to tomographic ultrashort pulse measurement, was called dispersoscopy. A patent for the *dispersoscopy* was granted in February 2014 [12]. The dispersoscopy is based on controlled spectral phase mod-



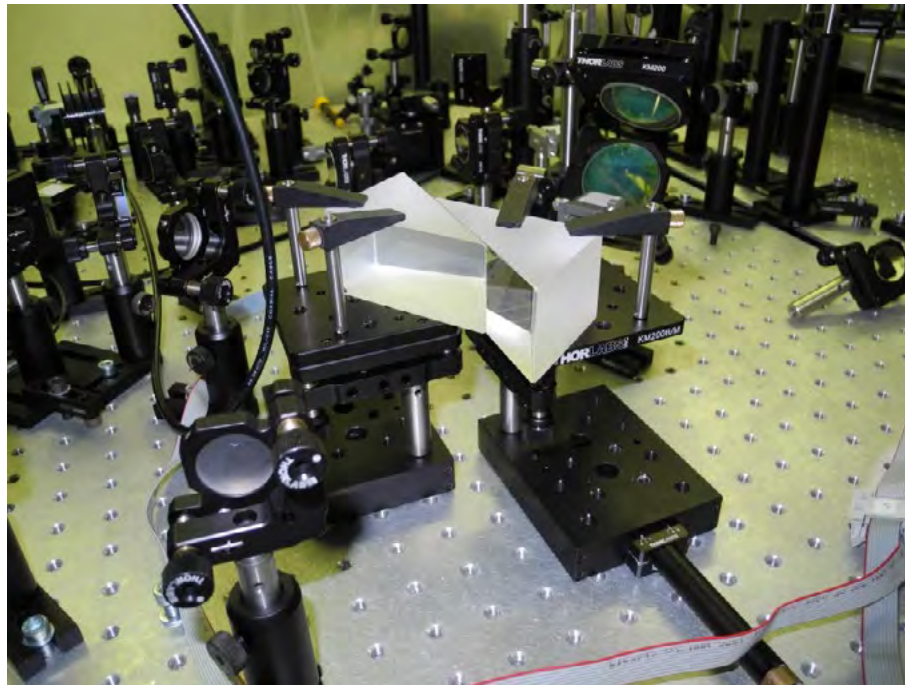


Fig. 5: Dispersive delay line

ulation of a measured pulse by a dispersive delay unit only and its detection by a temporally integrating spot detector. An optimizing algorithm enabling phase retrieval from a one dimensional experimental trace and an independently measured pulse frequency spectrum was also proposed and claimed in the patent. The dispersoscope has great potential to be modified for many spectral regions and ranges of pulse lengths. A particular configuration of a dispersoscope for measurement of fs pulses generated by a Ti:sapphire laser which was designed and carefully tested. In this pilot experiment, a special configuration of a dispersive delay unit which simply increases length of the measured beam path in optical glass was proposed (Fig. 5). Since the unique design of the dispersive delay unit is not only useful for dispersoscopy, this unit composed of two moveable right-angle optical prisms was claimed in another patent [13].

### kW-class, Pulsed Diode Pumped Solid State Lasers

Since 2012, one of the key points of research and development within the section are thin-disk based high-power picosecond lasers in the HiLASE Centre. The thin-disk geometry allows significant reduction of thermal lensing and should enable lasers to reach average power of 1 kW in picosecond pulses and fundamental spatial mode. Three thin-disk-based, kW-class laser beamlines are being developed [14], each de-

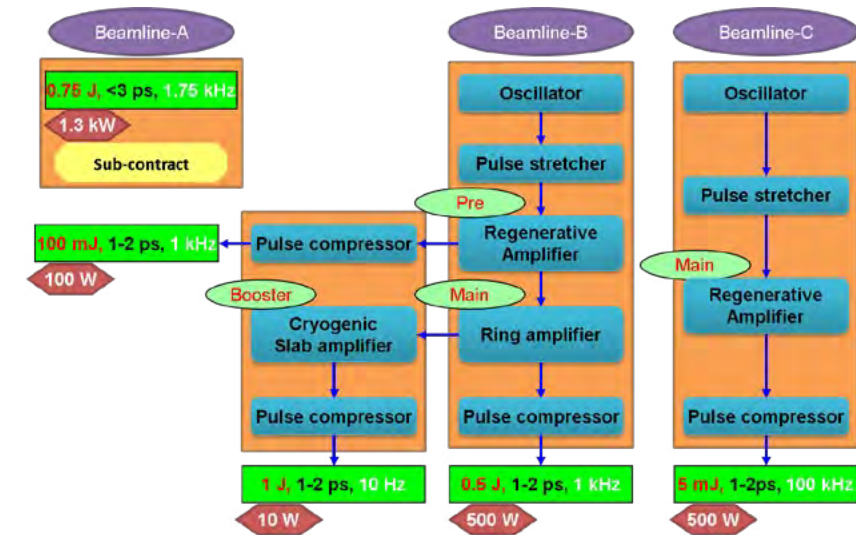


Fig. 6: Block scheme of thin-disk-based beamlines at the HiLASE Centre.

livering different output parameters (Fig. 6). Beamline A will deliver a 750 mJ pulse energy at a 1.75 kHz repetition rate. This beamline is subcontracted to Dausinger and Giesen GmbH in order to reduce the overall project risk associated with the high demands. The HiLASE research group is independently developing Beamlines B and C with output parameters of 500 mJ at a 1 kHz repetition rate and 5 mJ at a 100 kHz repetition rate, respectively. All beamlines will provide a pulse duration of 1–3 ps and have a potential of future upgrade to higher output power. The output of Beamline B can be diverted into a 120 Hz repetition rate cryogenic amplifier. Figure 6 shows block diagrams of our thin-disk laser beamlines.

Beamline A consists of a fiber front-end that includes a pulse stretcher, pulse picker, and optical isolator. The front-end produces laser pulses with an energy of 1 mJ at a repetition rate of 1.75 kHz. These pulses are further amplified in a regenerative amplifier to an energy of around 150 mJ, then in a linear amplifier to an energy of around 0.9 J. The amplified pulses are finally compressed in a grating pulse compressor down to about 3 ps. The whole laser system will be installed and commissioned in 2015.

Beamline B starts with an Yb-doped fiber oscillator at a central wavelength of 1030 nm with a bandwidth of more than 20 nm. Pulses from the fiber laser are stretched up to 500 ps. Afterwards, pulses are coupled into the regenerative amplifier cavity, amplified, and ejected through an optical isolator into a pulse compressor. 45 mJ picosecond pulses at 1 kHz repetition rate have been routinely generated in 2014. A schematic of the current status of Beamline B is shown in Fig. 7. In order to reduce thermally induced stress between the heatsink and the gain media, CuW is adopted as the heatsink material, because it has a similar linear expansion coefficient to YAG. The Yb:YAG crys-

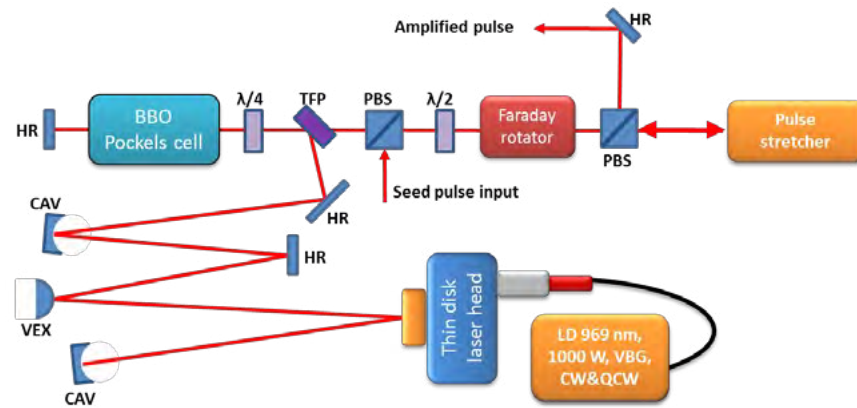


Fig. 7: Optical scheme of the first stage of the high-energy beamline B (500 mJ, 1 kHz).

tal is soldered onto the CuW heatsink using gold-tin solder. The amplifier is pumped by a novel scheme using a so called zero phonon line, pumping directly to upper laser level. A fiber-coupled diode laser module delivering an optical power of up to 1 kW at a wavelength of 969 nm is operated in a quasi continuous wave regime. Optimal pump pulse parameters were studied and set in order to minimize thermal loading of laser crystals [15]. The optical-to-optical efficiency was close to 20 %. The laser cavity is being upgraded with a second thin-disk head to reach an output energy of 100 mJ. Additionally, the Martinez-type stretcher is replaced with a fiber-chirped Bragg grating stretcher that enables better control of dispersion and is more stable and compact. Finally, the amplified pulses will be directed to a second regenerative amplifier that will be completed in 2014.

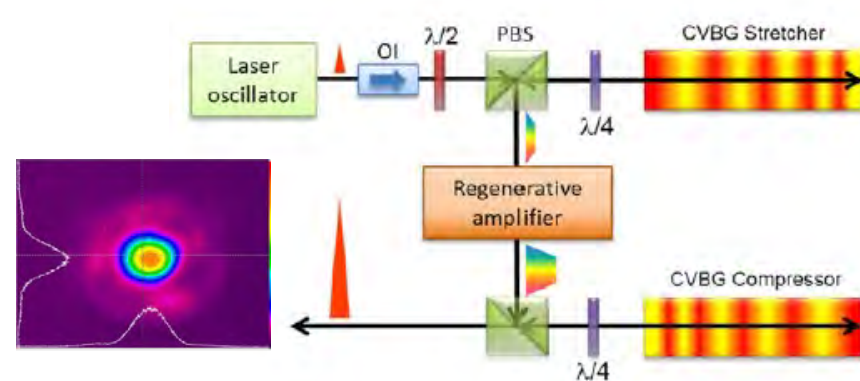


Fig. 8: Scheme of the compact high repetition rate beamline C (5 mJ, 100 kHz) employing a CVBG stretcher and compressor.

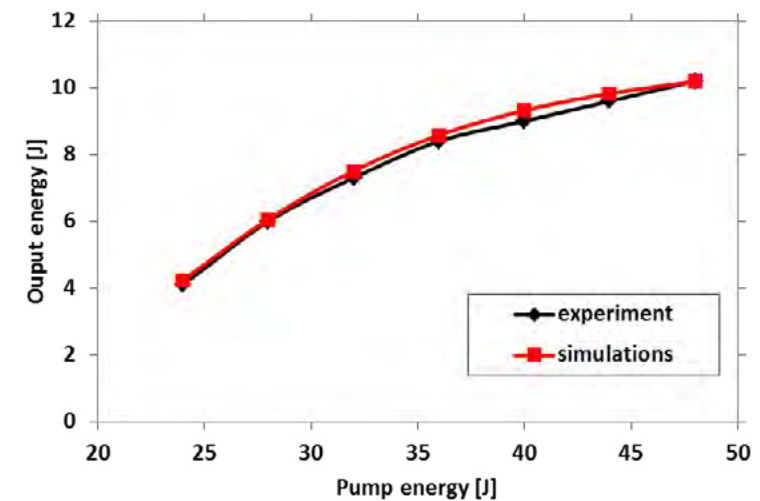


Fig. 9: Comparison of experimentally measured [17] and calculated output energy of 10 J cryogenic amplifier with different pump energy.

Beamline C is aimed at achieving a pulse energy of 5 mJ at a 100 kHz repetition rate. In order to meet these requirements, an intense study has been conducted to develop a high repetition rate regenerative amplifier. The target specifications of Beamline C will be achieved after completing three major milestones. The experimental setup for reaching the first milestone is shown in Fig. 8. Pulse energy of 0.8 mJ (compressed) at 100 kHz was achieved in 2014. The regenerative amplifier is seeded by an Yb-doped fiber oscillator, as in the Beamline B, but the pulses are stretched by a chirped volume Bragg grating (Fig. 8). A comparative study showing the advantage of zero-phonon-line pumping from the point of view of reducing thermal stress has been performed [16].

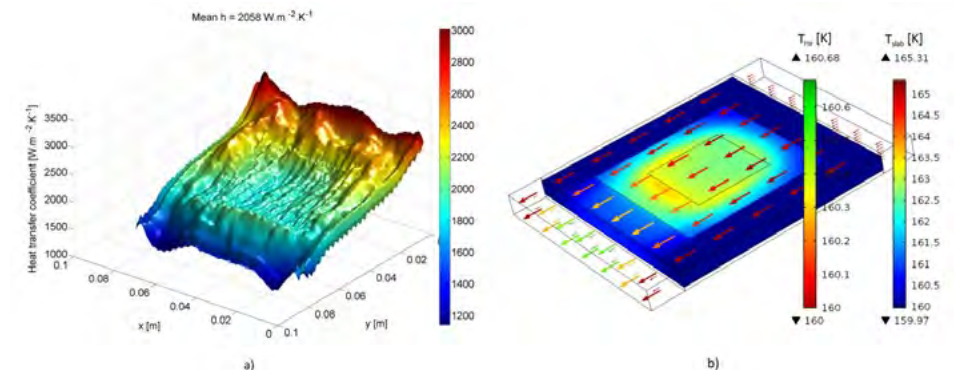
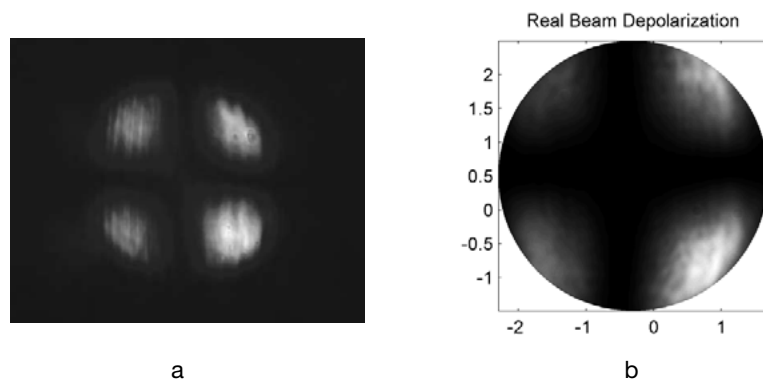


Fig. 10: (a) Heat transfer coefficient between He gas and surface of laser slab, (b) temperature map of the slab with scale for He gas (middle of the flow channel) and for slab surface [21].



A very compact chirped volume Bragg grating compressor was used allowing the system to be kept small and vibration resistant. The output pulse was compressed below 2 ps. The output energy will be further increased by using more intense pump light and by modifying the thin-disk head and the cavity. Technical difficulties connected to development of all the mentioned thin-disk beamlines are connected mostly to thermal management of the thin-disk modules and the availability of pump modules at a wavelength of 969 nm.

For efficient industrial utilization of novel materials, processing techniques that require high energy pulses (such as laser shock peening used to strengthen fatigue resistance of materials), new high energy lasers with high average power are required. These lasers will also find broad use in other areas including pumping of parametrical amplification of very short pulses for generation of ultra-high intensity pulses, testing large aperture optical elements for laser induced damage, or compressing fuel pellets in future fusion power plants. For pulsed lasers, the length of the amplifier cannot be easily extended because the energy must be stored in the amplifier for some time before it is released in the pulse. Large heat generation and thermal gradients in pulsed



**Fig. 11:** (a) Measured [10] and (b) calculated by HiLASE codes thermally induced depolarization in Faraday isolator

lasers introduce severe effects, such as thermally induced wavefront distortion and depolarization, that decrease the energy in the beam, the beam quality and can even lead to amplifier damage.

To design a high energy laser [17, 18], one needs to optimize pump intensity, generated heat, wavefront distortion, depolarization, and many other parameters. Complex computer codes have been developed and validated by the HiLASE team. We have developed code that calculates stored energy, output energy and heat generated in the laser amplifier with 3D resolution [19, 20]. The code takes into account the full geometry of the amplifier and its material parameters. Results of the code match experimental data obtained for 10 J Yb:YAG cryogenic amplifier very well, as shown in Fig. 9. Output of this code is then used to calculate stresses and temperature in the laser media for

prediction of depolarization [21] and wavefront deformation [22]. As an example, Fig. 10 shows the calculated heat transfer coefficient and temperature of the laser slab for an amplifier cooled by a flow of helium gas at very low temperature.

Our codes can also be used to calculate properties of other key elements of the laser system. One of such device is the Faraday isolator. Faraday isolators prevent scattered and residually reflected light from back-propagating in the amplifier chain and damaging the preceding amplifiers. For high average power lasers, the Faraday isolator heats up and its isolation is compromised due to thermally induced depolarization [23]. We have used our codes to accurately predict this depolarization for a large aperture Faraday isolator (Fig. 11) and the next step will be to optimize the design and improve the optical isolation. Having bespoke and reliable computer codes, we participate on the development of a new generation industrial laser with output energy of 100 J at a repetition rate of 10 Hz that is being built at STFC, Rutherford Appleton Laboratory, U.K. and will be installed at the HiLASE facility in Dolní Břežany in 2015.

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## Institute of Physics The Czech Academy of Sciences



## ELI Beamlines Project Division



## ELI Beamlines

The primary mission of the ELI Beamlines facility will consist of producing an entirely new generation of secondary sources driven by ultra-intense lasers and experimental stations dedicated to these sources, where future facility users will perform their experiments. The secondary sources will produce pulses of radiation and particles such as flashes of X-rays and gamma-rays, bunches of accelerated electrons, protons and ions, etc., exploitable as unprecedented research tools in many research disciplines and in the development of new technologies. The research agenda using the ultra-short and ultra-intense pulses delivered by ELI Beamlines is structured into six research activities: 1) Lasers generating ultrashort pulses and multi-petawatt peak power, 2) X-ray sources driven by ultrashort laser pulses, 3) Applications of X-ray sources in molecular, biomedical, and material sciences, 4) Particle acceleration by lasers, 5) Laser plasma and high-energy-density physics, and 6) Exotic physics and theory.

The outcomes of these six research activities during the years 2010–2014 will be briefly summarized in the following sections, followed by a short description of developments and the construction of the brand new ELI Beamlines building in Dolní Břežany, which will house all the research activities.

### Research Highlights

#### Lasers Generating High Repetition Rate Ultra-Short Multi-Petawatt Peak Power Pulses

The laser team of ELI Beamlines develops lasers systems and/or subsystems for the four high power laser systems of the ELI-Beamlines project. The facility will make available for users; high-brightness multi-TW ultrashort laser pulses at kHz repetition rate, PW 10 Hz repetition rate laser pulses, and kilojoule nanosecond laser pulses for generation of 10 PW peak power. These systems will meet the requirements of the international user community for cutting-edge laser resources for programmatic research in the generation and application of high-intensity X-ray sources, in particle acceleration, and in dense-plasma and high-field frontier physics. The ELI-Beamlines high repetition rate lasers now being developed will extensively employ the emerging technology of diode-pumped solid state lasers (DPSSL), to pump OPCPA (Optical Parametric Chirped Pulse Amplification) and Ti:sapphire short-pulse amplifiers.

An important auxiliary activity of the laser team is improvement, in cooperation with industry, of techniques of growing large crystals. A novel technology for the growth of large doped YAG crystals has been developed since 2011, which allows the production of highly homogeneous crystals without the central inhomogeneity, which is a char-



**Fig. 1:** Assembling the ps vacuum compressor for the L1 laser of ELI-Beamlines, designed by the Dept 91 research and technical team, in cooperation with engineering support by Dept. 93.

acteristic of the Czochralski technique. In 2014, a joint patent application FZU-Crytur for this technique was filed.

Other activities of the team involved design of a complex 5 m long compressor for 1 Petawatt L3 laser, pico second pumping lasers for the L1 kHz laser system and development of advanced laser diagnostics.

#### Selected publications and patents

- [1] F. Batysta, R. Antipenkov, J. Green, J. Naylor, J. Novák, T. Mazanec, P. Hříbek, C. Zervos, P. Bakule, and B. Rus: Pulse synchronization system for picosecond pulse-pumped OPCPA with femtosecondlevel relative timing jitter. *Optics Express* **22** (2014) 30281-30286.
- [2] D. Kramer, R. Barros, T. Medřík, J. Hřebíček, D. Peceli, M. Ďurák, M. Kozlová, B. Rus: Commissioning and first results of the ELI-beamlines LIDT test station. *Proceedings of SPIE* **8885** (2013).
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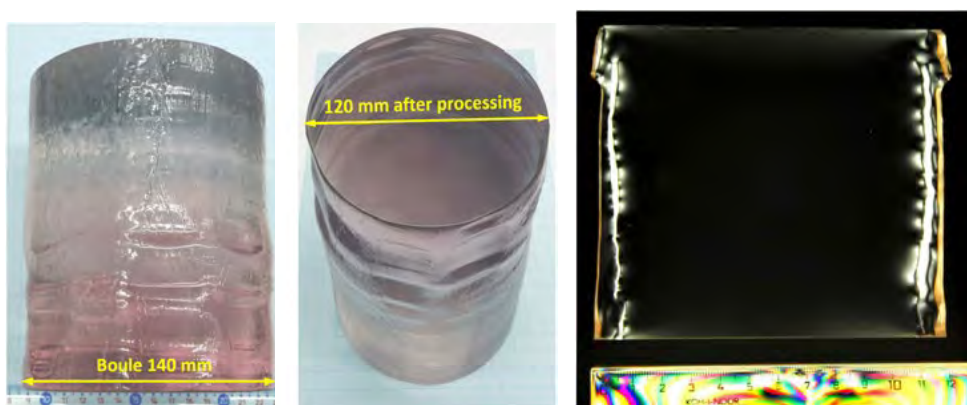
## X-ray Sources Driven by Ultra-Short Laser Pulses

One of the main goals of this research activity is to develop sources of ultrashort X-ray pulses, both coherent as well as incoherent, paving the way towards imaging nature with atomic resolution both in space and time with university-lab sized devices. The laser-based sources have, in contrast to large-scale facilities such as third-generation synchrotrons or X-ray Free-Electron-Lasers (XFELs), spanning distances of hundreds of meters, their great advantage being these are only university-lab sized and can, thus, offer a much broader accessibility as only few large-scale facilities exist world-wide.

### Investigation of laser driven coherent soft X-ray beams

Soft-X-ray lasers (SXRL) and High order harmonics (XRL) have been proven to be tools of great interest for practical applications. The main activities of the group on X-ray lasers included source development and applications in dense plasma diagnostics, warm-dense matter generation, fusion, relevant plasmas studies, investigations related to astrophysics in laboratory, and holographic microscopy.

Recently, research was oriented towards high-repetition rate sources of XUV radiation as high-order harmonic generation with quasi-phase matching to enhance the conversion efficiency and the design of dedicated HHG beamline that will be constructed in the E1 hall of the ELI Beamlines facility. The goal parameters should be achieved at different stages of the kHz laser development. The actual design includes a two-colour driver ( $\omega$  and  $2\omega$ ) to improve the conversion efficiency. This technique generates even and odd harmonics and the conversion efficiency can be significantly increased up to  $10^{-3}$ . A few  $\mu\text{J}$  of coherent EUVs are thus expected per shot at kHz rep-

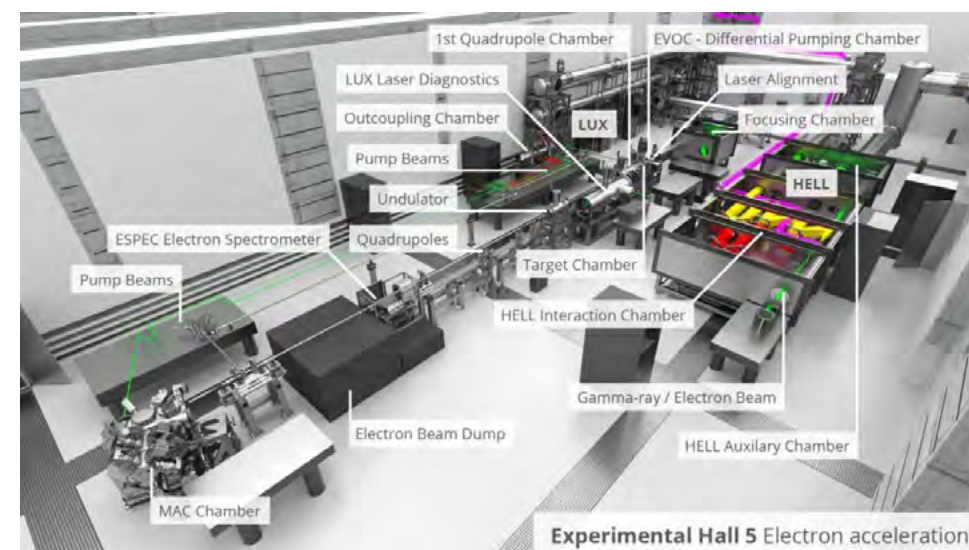


**Fig. 2:** Yb: YAG laser monocrystals (Yb doping 2%) with a diameter of 14 cm, grown by novel technology developed in FZU in cooperation with Crytur Ltd. company. It is the largest YAG monocrystal of this type in the world. The image on right shows a 10x10 cm slab vertically cut from the monocrystal in crossed polarizers demonstrating its excellent optical quality (note image of the plastic ruler in the crossed polarizers).

etition rate. Moreover, we can take advantage of the high energy of the laser driver and of the large size of the room to set extra-long focal length geometry. Shorter focusing will be available to generate reasonable EUV photon fluxes at lower laser energies or to generate shorter wavelength radiation.

Furthermore the following harder X-ray sources and new concepts of short (a few fs-long) soft X-ray beamlines were being developed and their technical design has advanced significantly:

- **1. kHz repetition rate X-ray plasma source**, few 1/10ths of a keV using a laser driven plasma as the emitter.
- **2. Betatron beamline**, using laser accelerated electrons wiggling in a miniature magnetic chicane created inside a plasma channel and producing X-ray photons with energy in keV range.
- **3. Laser-driven undulator X-ray source (LUX)** accelerating electrons and forcing them to emit soft X-ray photons by slaloming in a periodic permanent magnet structure called an undulator. This beamline is developed in collaboration with the University of Hamburg and a significant effort was put both into its conceptual physics design and technical implementation.
- **4. Compton source**, colliding short pulse lasers with laser driven electrons, 100 keV to MeV range



**Fig. 3:** A visualization of 3D technical design of LUX beamline and electron accelerating HELL beamline within experimental hall E5.



## Selected publications

- [1] F. Tissandier, S. Sebban, M. Ribière, J. Gautier, Ph. Zeitoun, G. Lambert, J-Ph. Goddet, F. Burgy, A. Rousse, J. Nejd, T. Mocek and G. Maynard: Bessel spatial profile of soft x-ray laser beam. *Applied Physics Letters* **97** (2010) 231106.
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- [3] J. Nejd, M. Kozlová, T. Mocek, and B. Rus: Measuring the electron density gradients of dense plasmas by deflectometry using short-wavelength probe. *Physics of Plasmas* **17** (2010) 122705.
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- [5] L. M. R. Gartside, G. J. Tallents, A. K. Rossall, E. Wagenaars, D. S. Whittaker, M. Kozlová, J. Nejd, M. Sawicka, J. Polan, M. Kalal, and B. Rus: Extreme ultraviolet interferometry of warm dense matter in laser plasmas. *Optics Letters* **35** (2010) 22.
- [6] D. Batani et al.: Generation of high pressure shocks relevant to the shock-ignition intensity regime. *Physics of Plasmas* **21** (2014) 032710.

## Applications of X-ray Sources in Molecular, Biomedical and Materials Sciences

This group is building up the experimental capabilities within ELI Beamlines, enabling the users to study their samples probed by X-ray sources in dedicated experimental chambers connected to the sources. The research has been performed with partner institutions or other world leading centres in photon based sciences. This research is concentrated on different aspects of future Beamlines implementations including the training of new team members. Recently, members of this research activity have performed experiments in the associated fields of materials and nano-science, structure and dynamics in solids and characterization of high intensity laser-matter interactions. The following areas and capabilities have been identified and the development and procurement of the required instrumentation has been initiated:

- **1. Coherent Diffractive Imaging (CDI) and Atomic, Molecular and Optical (AMO) Science:** Performed in a multi-purpose vacuum chamber at either the HHG source or the LUX beamline. Sample delivery techniques will cover gas, cluster, aerosol and liquid jet sources as well as solid targets. Detectors will be available for imaging, as well as for photon, ion and electron spectroscopy.
- **2. Soft X-ray Materials Science:** This research will be supported by a unique ellipsometer for time-resolved magneto-optical ellipsometry in the VUV range (10 to

40 eV). The instrument will have a sample holder with a closed cycle cryostat and a +/- 1.5 T magnetic field that is switchable with the 1 kHz rep rate of the L1 laser.

- **3. Hard X-ray science, diffraction, spectroscopy and imaging:** Implemented in a modular experimental area served either by the laser driven plasma X-ray source or the Betatron source. Detectors will include a high read out rate Mpixel detector capable of reading out at the 1 kHz rep. rate of the L1 laser.
- **4. Optical Spectroscopy and pump beams:** This work package will serve all X-ray beamlines for applied sciences with pump beams for advanced pump-probe experiments. Pump beams will be generated from the THz range up to 180 nm (also to a pulse duration as short as 5 fs) covering delays from fs to ms. The area for the generation of pump beams will also be capable of advanced spectroscopy studies in the IR to UV range, most notably the development of Stimulated Raman Spectroscopy for applications in molecular dynamics and pulse radiolysis.

## Selected publications

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- [4] T. Burian et al.: Soft x-ray free-electron laser induced damage to inorganic scintillators. *Optical Materials Express* **5** (2015) 254-264.
- [5] A. Zelenakova, V. Zelenak, S. Michalik, J. Kovac and M. W. Meisel: Structural and magnetic properties of CoO-Pt core-shell nanoparticles. *Physical Review B* **89** (2014) 104417.
- [6] A. Rath et al.: Explosion dynamics of sucrose nanospheres monitored by time of flight spectrometry and coherent diffractive imaging at the split-and-delay beam line of the FLASH soft X-ray laser. *Optics Express* **22** (2014) 28914.

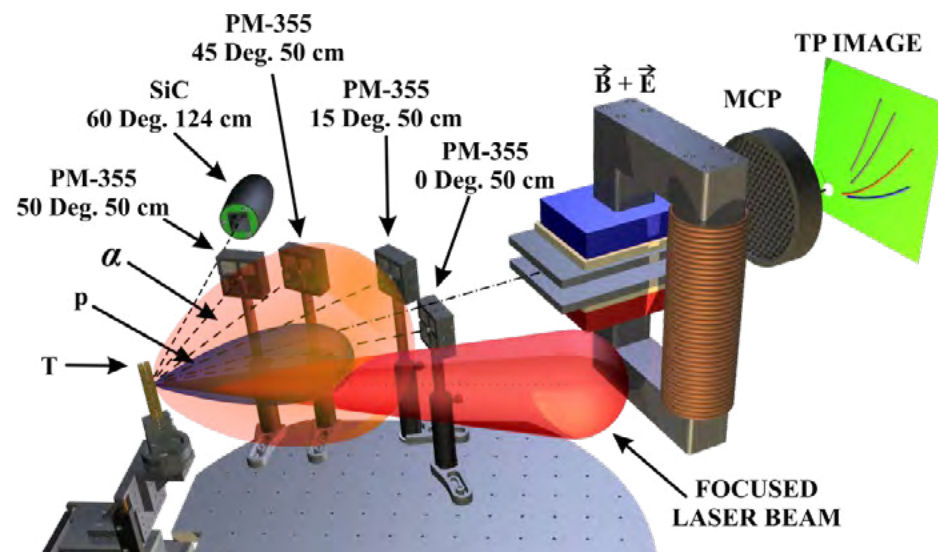
## Particle acceleration by lasers

The main research results of this research activity during the evaluated period are illustrated by two publications in journals with high impact factor dedicated to laser-driven proton acceleration and Boron-Proton nuclear fusion enhancement; and by one patent related to enhancement of nuclear fusion and awarded within the evaluated period.

- Laser-Driven Proton Acceleration Enhancement by Nanostructured Foils  
*Physical Review Letters* **109** (2012) 234801

Laser driven ion acceleration is a very promising approach which might significantly reduce the typical size and cost of standard acceleration systems used for example for hadron therapy of tumours. Nevertheless the laser accelerated beams have to be improved in terms of energy, current, divergence, shot-to-shot stability, etc. In a recent experimental campaign our team has greatly improved both the maximum energy (about 60%) and number (approximately 5 times) of the proton source by using a high intensity laser and advanced nanostructured targets.

This is the first theoretical and experimental proof of an enhanced TNSA (Target Normal Sheath Acceleration) regime. Using a special technique, sub-micron spheres with diameters close to the wavelength (or slightly smaller) are placed on the front side of a thin target. This leads to an increase of laser light absorption and connected with this an enhancement of the hot electron population and temperature, thus leading to a more efficient acceleration (higher energy and number of accelerated protons).



**Fig. 4:** Experimental setup used in the paper “Boron-Proton Nuclear-Fusion Enhancement Induced in Boron-Doped Silicon Targets by Low-Contrast Pulsed Laser”

This result was achieved in cooperation with the scientific teams working at the PW-class APRI-GIST laser facility in South Korea and at the Czech Technical University in Prague. The projection of such a result towards higher laser intensities seems to be very promising for the application of laser accelerated particle beams in various societal fields, e.g. the design of new hadron therapy centres for cancer treatment.

- Boron-Proton Nuclear-Fusion Enhancement Induced in Boron-Doped Silicon Targets by Low-Contrast Pulsed Laser  
*Physical Review X* **4** (2014) 031030

Currently laser-induced nuclear fusion reactions are being investigated for their potential use as alternative energy sources for society. Nuclear fusion involving boron has garnered interest since the 1930s when it was investigated by Oliphant and Rutherford because of its ability to produce copious numbers of alpha particles, which can in turn be used for generating fusion energy without production of neutrons.

Our papers show a clear enhancement of the  $^{11}\text{B}(p,\alpha)^2\alpha$  fusion reaction yield by using modest laser intensities and advanced multi-layer targets. A fusion rate of  $\sim 10^9$  alpha particles per steradian per pulse was achieved by using boron-hydrogen enriched silicon targets. This result is ascribable to the high proton yield generated by the long (nanosecond) laser pulse, which presented an optimal energy spectrum with a plateau around the maximum of the nuclear reaction cross section.

The advantage of our proposed experimental method lies in the use of a moderate laser power (2 TW) and intensity ( $3 \times 10^{16} \text{ W.cm}^{-2}$ ) that could possibly in the future enable the use of compact laser systems and simple irradiation geometries. Our approach does not require special laser techniques for compressing the pulse such as the chirped pulse amplification method; thus, a less sophisticated and cheaper system is sufficient.

Furthermore, preliminary hydrodynamic simulations suggest that the relevant physical mechanisms which enable such high yield fusion reactions can occur with lower laser energy. Thus, in principle, this scheme can be realized using small and cost-effective laser systems (tens of joules, nanosecond-class and high repetition rate), for instance based on newly established diode-pumped laser technology, which might pave the way for more advanced technological applications.

## Selected publications

- [1] D. Margarone, A. Picciotto, A. Velyhan, J. Krasa, M. Kucharik, A. Mangione, A. Szydlowsky, A. Malinowska, G. Bertuccio, Y. Shi, M. Crivellari, J. Ullschmied, P. Bellutti, G. Korn: Advanced scheme for high-yield laser driven nuclear reactions. *Plasma Physics and Controlled Fusion* **57** (2014) 014030.
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## Plasma and High Energy Density Physics

This research activity tackles behaviour of matter and plasma under extreme temperatures and pressures (or strong electro-magnetic fields) which in nature appear in the cores of massive planets such as Jupiter, in brown dwarfs and in stars. The field also includes experiments with plasma as the amplifying medium for laser pulses and other topics described below. Let us also note that apart from the experimental activities described below, the team has also strongly focused on the physics and technical design of a large experimental platform enabling such experiments at ELI Beamlines under even more extreme – and more interesting – conditions, including the 10 Petawatt laser flagship.

### Plasma amplification experiments

The first successful proof-of-principle experiment for ion-wave based plasma amplification was carried out in 2010 using the ELFIE laser system of the LULI laboratory. Subsequent experimental campaigns optimized the set-up, the interaction conditions and the geometry. In the latest experiment a head-on collision between pump and seed was performed. Absolute amplification and large energy transfers were obtained. Plasma amplification provides in the long-term the potential to overcome present limitations to increase the focused intensity of light pulses. Plasma amplification as well as plasma focusing is part of the growing field of plasma optics which can cope with

very high energy densities and responds to the present technological and scientific needs of high-field science.

### X-ray spectroscopy of laser-matter interaction

The plasma produced by the interaction of sub-ns laser pulses was studied in wide experimental collaborations as a possible medium for achieving the inertial confinement fusion. X-ray spectroscopy provided information about the plasma parameters and thus the interaction phenomena such as shock wave generation and laser ablation were studied in well-defined environments. In another experiment, the generation of collimated plasma jets and their consequent collision with secondary targets was studied, providing information about the plasma-solid interactions. The acceleration of electrons via laser irradiation of solid targets and their propagation in plasmas was diagnosed via the collision induced  $K\alpha$  radiation, both with sub-ns and fs lasers. Concerning the studies of atomic physics, the charge-exchange process was experimentally observed, and the atomic processes accompanying isochoric heating of material irradiated by the high-intensity X-ray free electron laser radiation were studied via the radiation driven K-shell emission. X-ray imaging can be used in an efficient way to image hot electrons.

### Equation of state under warm dense matter conditions

A new approach to equation of state experiments, based on a laser-driven shock and release technique combined with spatially resolved X-ray Thomson scattering, radiography, velocity interferometry, and optical pyrometry, to obtain independent measurements of pressure, density, and temperature for carbon at warm dense matter conditions. The uniqueness of this approach relies on using a laser to create very high initial pressures to enable a very deep release when the shock moves into a low-density pressure standard. This results in material at near normal solid density and temperatures around 10 eV. The spatially resolved Thomson scattering measurements facilitate a temperature determination of the released material by isolating the scattering signal from a specific region in the target. Our results are consistent with quantum molecular dynamics calculations for carbon at these conditions and are compared to several equations of state models.

### Selected publications

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- [3] D. Batani et al.: Generation of high pressure shocks relevant to the shock-ignition intensity regime. *Physics of Plasmas* **21** (2014) 032710.
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- [5] M. Šmíd et al.: Investigation of x-ray emission induced by hot electrons in dense Cu plasmas, *Physica Scripta* **T161** (2014) 014020 (2014)
- [6] K. Falk, E.J. Gamboa, G. Kagan, D.S. Montgomery, B. Srinivasan, P. Tzeferacos, J.F. Benage: Equation of State Measurements of Warm Dense Carbon Using Laser-Driven Shock and Release Technique. *Physical Review Letters* **112** (2014) 155003.

### Exotic physics, theory, simulation & computing

This team has focused on the following activities:

#### Tight focusing analysis and subsequent electron dynamics

How to focus a multi-petawatt laser pulse to very high intensities is a major issue for all the forthcoming 10PW installations such as ELI-Beamlines. Small focal length parabolas cannot be used easily due to potential damage and debris production. A possible solution is to perform tight focusing with a combination of an off-axis parabola in conjunction with an ellipsoidal plasma mirror. This will allow the attainment of intensities in the focal spot above  $10^{23}$  W/cm<sup>2</sup>. However, for these extreme conditions the standard paraxial approach breaks down and a direct integral approach to Maxwell's equations has to be used. In the focal spot a longitudinal electric field develops. This strongly affects the motion of electrons as it is exposed to the ponderomotive forces in the longitudinal and transverse directions as well as the longitudinal field. At these high intensities the radiation-reaction force needs to be taken into account. Such a setup will eventually allow the study of extreme relativistic and quantum effects of electron motion.

#### Shock-ignition approach to inertial confinement fusion

The shock-ignition (SI) approach to inertial confinement fusion (ICF) attempts to overcome certain deficiencies of the standard direct or indirect drive. However, as it operates at a much higher intensity than is normally employed in ICF, parametric instabilities play a major role. Laser-plasma interaction for SI is still little studied and the issue of laser energy absorption and preheat are still of major concern. Large-scale, multi-dimensional kinetic simulations on long time scales provide answers to these open questions.

#### Theoretical and simulation analysis of plasma amplification

The quest for ever higher focused laser intensities is limited by the damage threshold of solid-state based optical materials and the size of gratings that can be easily man-

ufactured. A new approach for creating short and intense laser pulses is based on the collision of a relatively long pump pulse of low intensity with a short seed pulse inside plasma. The two transverse modes are coupled by a longitudinal plasma mode (in the present case an ion-acoustic mode in the strong-coupling regime) which allows the energy transfer from the pump to the seed. As the duration of the final pulse is given by the seed, the energy transfer implies a considerable increase in intensity.

The work of the team was also focused on laboratory astrophysics and radiation-reaction and pair creation at ultra-high intensities.

### Selected publications

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### ELI Building

#### Construction steps

An architectural competition for the ELI building was held in 2009 resulting in the development of the initial plans for the ELI centre. The contract of delivering the full project documentation for the building's construction was signed with the British company Hamiltons, the author of the winning study. To build such a large object in the centre of the village, local authorities had to adjust their local civic plans. The first design work for planning and building permits were made between 2010 and 2012.

The geological and hydrological survey, negotiations on land redemptions from the original owners (the Prague Archdiocese and a former Cooperative farm), land survey and other preliminary works on the technical network took place simultaneously with





Fig. 5: Visualization of the ELI building

the design process. A second activity was the coordination of the ELI project with its neighbour project, HiLASE and the planned reconstruction of the area behind the town hall.

At the end of 2011, we divided the construction into two phases. The tender documentation for each phase was prepared separately to allow the choice of two general suppliers and to reduce the risk of tender failure. The tender documentation was based on the detailed execution documentation provided by the architectural office, which had been meanwhile renamed as Bogle Architects.

The *Preliminary phase* included knocking down of the existing, derelict buildings, the area-wide archaeological survey, which was extended due to a number of valuable discoveries, but above all the digging out a large excavation pit (90ths. m<sup>3</sup> of soil) and its stabilisation, which required the compacting of almost vertical walls with a spread concrete. This action took place from June 2012 until May 2013 and was carried out by the company Strabag.

The second, *Main phase* has followed smoothly. This included the construction of the building's themselves. These are being finalized at present. From the beginning, this phase was split into Work 1 (administration building and the separate building containing the plant room for cooling and technical gases in the street Ke dvoru) and Work 2 (the laser hall with laboratory building). It was planned that Work 1 would be finished before the finalization of the laser hall. This has been achieved and work in the office building started in July 2015. This phase is carried out by an association of 3 companies MVO (Metrostav, VCES, OHLŽS).

The building activities in Dolní Břežany were affected by the heavy rains in the spring 2013, which partly damaged the securing of the excavation pit and slowed down the start of the *Main phase* of the construction overall. The weather (two mild winters) has been favourable since then.

### Description

The ELI building consists of two functionally interconnected buildings, the Administration building (the northern part of the building) and the Laser building (the southern part of the building) which provides in particular research halls and laboratories. There are about 300 employees and 50 external workers.

**The Laser hall** is a unique monoblock made from the cast concrete. Specific requirements for its volume, space rigidity and shading parameters has necessitated a unique recipe of heavy and very firm concrete to be used to build the massive walls and ceilings with a thickness of up to 1.6 meters. The building had to be established on maximally stable rocky subsoil no vibrations or unbearable foundation cleft could endanger the stability of the interior. Maximal thermal stability in the building was also required, so the building is partly recessed into the ground. A major feature of the building is the housing of hi performance cooling and heating devices. Each floor in the laser hall is double height (7.5m k.v.) to provide enough space for the installation of laser technologies. The building is topped by a green roof,

**The Laboratory building** functions as a base for preparation and service. From this place – central control rooms will manage all laser activities. On the upper floor there are offices to rent for incoming users.

**The Administration building** includes offices, a multifunctional area, meeting rooms and the vestibule. The Office building mostly houses offices for 1-4 persons. The maximum capacity of one office is 8 persons. There are three internal atriums which bring light to the central area of building, creating a very pleasant working environment.

The multi-purpose building houses a canteen, lecture hall for an audience of 150, schoolrooms (one of these for 40 persons) and three lounges (each for 20 persons).

A dining hall with kitchen for warming up delivered meals is in the middle of the 1st floor. Catering services will be provided by an external company on a contract basis. The dining hall is located on two floors which are connected by a staircase, there are additional seats. Next to the dining hall are the meeting room with possible catering services, the school room and the lecture hall with interpreter booth.

### ELI Beamlines Prospective Impact

The ultrashort and ultra-intense pulses of light and particles will find many applications in fundamental research and in chemistry, biology, medical technologies, and the development of new materials. In fundamental research, for the first time it will be possible to study the phenomena connected to, quantum electrodynamics, space-time dependent radiation fields, structure of vacuum, etc., in the laboratory. Furthermore, it will help in the understanding the astrophysical phenomena involved in mechanisms of

radiation emitted by pulsars, brown dwarfs, and giant planets etc.. In the field of practical applications, the new laser-driven sources will enable significant improvements in screening techniques in medical diagnostics, and the capability of ultrashort pulses to provide high-resolution snapshots of molecules will contribute to better understanding of complex diseases such as cancer, and will enable development of personalized medicaments and medical treatments. The capability of ultrashort light pulses to obtain snapshots that have been thus far inaccessible and the “freezing in time” of physical materials and chemical molecules will help the development of new materials for electronics, optoelectronics, nanotechnologies, and many others.

The ELI facility will also create an attractive platform to develop a new generation of PhD students, scientists and engineers. This will significantly increase the visibility of the host country, the Czech Republic and of the cutting edge research facility and will attract further investments in advanced technologies.

ELI Beamlines will provide 250 workplaces and will host about 50 visiting researchers at a time.





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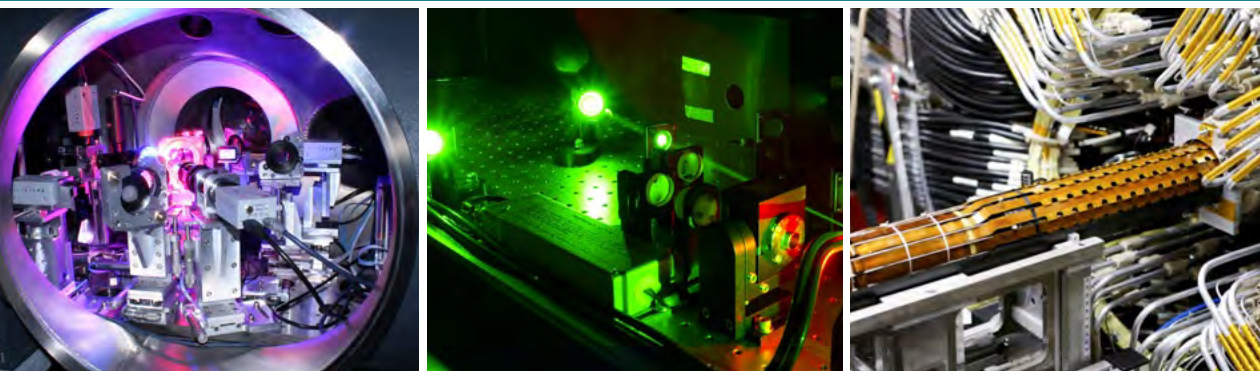
# Additional Information

The Czech Academy  
of Sciences



Institute of Physics  
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Prominent Personalities  
of the Institute History



## Prof. Ing. Jiří Niederle, DrSc.

**\*1939 – †2010**

An outstanding researcher in the field of mathematical physics and particle physics, especially the theory of gauge fields. After 1990, as a chairman of the Council for Foreign Relations of the Academy of Sciences, he significantly contributed to the substantial expansion and improvement of international scientific collaboration of the Academy. He was the first representative of the Czech Republic in the NATO Science Committee and the first representative of Czechoslovakia and later the Czech Republic in CERN – the European Organisation for Nuclear Research; he significantly contributed to admission of the Czech Republic to CERN, where he was three times elected vice president of the CERN Council.



## Prof. Ing. Dr. RNDr. Jan Tauc, DrSc.

**\*1922 – †2010**

One of the founders of solid state physics in the Czech Republic and a world-renowned researcher in the field of semiconductors: in cooperation with Z. Trousil he created the first germanium transistor outside of the United States. In the Institute of Technical Physics in Cukrovarnická street (later the Institute of Solid State Physics, today a part of the Institute of Physics) he founded and led the Department of Semiconductor Physics that linked basic physical research with the then-developing field of material research. He was engaged in research of the generation of electromotive forces in semiconductors and discovered the photovoltaic effect, anomalous thermal effect, photomagnetic effect and photopyroelectric effect; he significantly contributed to the study of inter-band transitions by means of optical measurement.



## RNDr. Svatopluk Krupička, CSc.

**\*1922 – †2014**



A pioneer in the research of magnetic properties of oxide materials of classic and new types, especially ferrites, garnets and perovskites. Director of the Institute of Physics during the critical four years after the Velvet Revolution in 1989. He established and managed the fundamental reorganization of the Institute, resulting in the formulation of new scientific challenges and new methods of evaluation that led to significant development of scientific research.

## RNDr. Leoš Láška, CSc.

**\*1938 – †2013**



A pioneer in the research of laser ion sources, especially highly ionized heavy elements. He was a leader of the working group that designed and built a two-stage amplifier of the iodine photodissociation laser PERUN. This started systematic research of laser-generated plasma in the Czech Republic, in laboratories PERUN, PALS (Prague Asterix Laser System) and subsequently to inform the needs of the emerging infrastructure ELI Beamlines. The South Italian regional conference on physics of laser plasma PPLA (Plasma Physics and the Laser Applications) has awarded the “Leos Laska Award” for the best young researchers of local universities since 2013.

## RNDr. Vladimír Dvořák, DrSc.

\*1934 – †2007

One of the most outstanding personalities of Czech physics, and from 1995 a member of the Learned Society, he was extremely talented, gifted with an excellent memory. Since the beginning of his scientific career he had been very active, not only in his scientific work, but also as a man – sportsman, he was an avid tennis player. He dealt with the theory of ferroelectric materials and structural phase transitions, but with the talent to explain clearly very complex physical phenomena. He developed e.g. the classification of structural phase transitions from the view of the symmetry of the order parameter in the form of detailed tables. By this, he founded the entire school and methodology to analyze temperature anomalies of various quantities in the vicinity of phase transitions. He was also engaged in the study of quasicrystals and other brand new metamaterials. Both his career and private life were linked with the Institute of Physics – he met his wife Hana here. Between 1993–2001 he worked as a director of the Institute of Physics. In his honour the Institute annually organizes a festive Dvorak lecture delivered by an internationally recognized authority (more on p. 29).



## Prof. RNDr. Jan Fousek, DrSc.

\*1930



One of the founders of physics of ferroelectrics in the Czech Republic; as a longtime head of the Department of Physics of Dielectrics of the Institute of Physics he contributed to construction of a unique laboratory of dielectric spectroscopy aimed at clarifying phase transitions in solids and liquid crystals. He organized the first International Meeting on Ferroelectrics (IMF, Prague, 1963). These conferences are regularly held to this day.

## RNDr. František Kroupa, DrSc.

\*1925 – †2009

A world-renowned expert in the theory of dislocation, popular among his colleagues, a passionate athlete, paddler, skier and above all an honest man. In his extensive scientific and pedagogical activities he introduced physical methods of material research; his frequently-cited work ranged from the theory of elastic continuum through mesoscopic models of dislocation cores to the atomic approaches to crystal distortions. From his results we highlight here the mathematical description of dislocation loops, spatial breakdown of dislocation cores resulting in poor flexibility or fracture processes in ceramic materials. In the critical year of 1968 he was first awarded the State Prize of Klement Gottwald. However, as a corresponding member of the Academy, he strongly protested against the Soviet invasion and especially against the normalization of AV management thus he was consequently forced to leave the Academy of Sciences. He returned to basic research five years later at the Institute of Plasma Physics. Soon after the establishment of the Institute of Physics he founded the Department of Mechanical Properties of Solids that changed its orientation through the study of metal physics to the present-day progressive structural materials. In the years 1966–1970, he worked as a senior editor at the Czechoslovak Journal of Physics dedicating his focus to the English version of the Journal.







Institute of Physics  
The Czech Academy  
of Sciences

Top Publications

## The Most Cited Publications of All Time

The publications were selected in order to illustrate the broad spectrum of research carried out at the Institute of Physics.

Title	Author(s)	Citations
Circular Edge Dislocation Loop Czechoslovakij fiziceskij zurnal B 10(4) 284–293 (1960)	F. Kroupa	137
Optical Properties and Electronic Structure of Amorphous Germanium Phys. Status Solidi 15(2) 627–637 (1966)	J. Tauc, R. Grigorovici, A. Vancu	2813
Single-site Approximations in the Electronic Theory of Simple Binary Alloys Phys. Rev. 175(3) 747 (1968)	B. Velický, S. Kirkpatrick, H Ehrenreich	1240
Improper Ferroelectrics Ferroelectrics 7(1-4) 1–9 (1974)	V. Dvořák	135
Theory of Quantised Hall Conductivity in Two Dimensions J. Phys. C Solid State 15 L717–L721 (1982)	P. Středa	412
Generalized Kadanoff-Baym Ansatz for Deriving Quantum Transport Equations Phys. Rev. B 34(10) 6933–6942 (1986)	P. Lipavský, V. Špička, B. Velický	262
Edge states, Transmission Matrices and the Hall Resistance Phys. Rev. Lett. 59(17) 1973–1975 (1987)	P. Středa, J. Kučera, A. MacDonald	221
Strings on World-Sheet Orbifolds Nucl. Phys. B 327(2) 461–484 (1989)	P. Hořava	265
The Prague Laser Asterix System Phys. Plasm. 8(5) 2495–2501 (2000)	K. Jungwirth, A. Cejnarová, L. Juha et al.	225

Title	Author(s)	Citations
Wide Band Gap Scintillation Materials: Progress in the Technology and Material Understanding Phys. Status Solidi A 178(2) 595–620 (2000)	M. Nikl	310
Universal intrinsic spin Hall effect Phys. Rev Lett. 92(12) 126603 (2004)	J. Sinova, D. Culcer, Q. Niu et al.	1121
Experimental Observation of the Spin-Hall effect in a Two-dimensional Spin-orbit Coupled Semiconductor System Phys. Rev. Lett. 94(4) 047204 (2005)	J. Wunderlich, B. Kaestner, J. Sinova et al.	817
Hardness of covalent and ionic crystals: First-principle calculations Phys. Rev. Lett. 96(8) 085501 (2006)	A. Šimůnek, J. Vackář	174
Theory of Ferromagnetic (III,Mn)V Semiconductors Rev. Mod. Phys. 78(3) 809–864 (2006)	T. Jungwirth, J. Sinova, J. Mašek et al.	754
Correlation of the Highest-energy Cosmic Rays with Nearby Extragalactic Objects Science 318(5852) 938–943 (2007)	Pierre Auger Collaboration	451
SUPERFLIP – a Computer Program for the Solution of Crystal Structures by Charge Flipping in Arbitrary Dimensions J. Appl. Crystallogr. 40 786–790 (2007)	L. Palatinus, G. Chapuis	932
Observation of a New Particle in the Search for the Standard Model Higgs Boson with the ATLAS Detector at the LHC Phys. Lett. B 716(1) 1–29 (2012)	ATLAS Collaboration	2759

Note: Citation volumes vary across various research fields thus the numbers in the last column are not mutually comparable. Publications are ordered by year of publication.



## The Most Cited Publications of Last Five Years

The publications were selected in order to illustrate the broad spectrum of research carried out at the Institute of Physics.

Title	Author(s)	Citations
In Situ Neutron Diffraction Investigation of Deformation Twinning and Pseudoelastic-Like Behaviour of Extruded AZ31 Magnesium Alloy Int. J. Plasticity 25(6) 1107–1127 (2009)	O. Muransky, D. G. Carr, P. Šittner et al.	84
Tunable Terahertz Metamaterials with Negative Permeability Phys. Rev. B 79(24) 241108 (2009)	H. Němec, P. Kužel, F. Kadlec et al.	49
Anisotropy of Hardness from First Principles: The Cases of ReB <sub>2</sub> and OsB <sub>2</sub> Phys. Rev. B 86(6) 060103 (2009)	A. Šimůnek	42
Turning Solid Aluminium Transparent by Intense Soft X-Ray Photoionization Nat. Phys. 5(9) 693–696 (2009)	B. Nagler, U. Zastraub, R. R. Faustlin et al.	132
Magnetocrystalline anisotropies in (Ga,Mn)As: Systematic theoretical study and comparison with experiment Phys. Rev. B 80(15) 155203 (2009)	J. Zemen, J. Kučera, K. Olejník et al.	46
A Simple Analytic Solution for Tachyonic Condensation J. High Energy Phys. 10(066) (2009)	T. Erler, M. Schnabl	45
Grain Boundary Segregation in Metals Springer (2010)	P. Lejček	118

Title	Author(s)	Citations
Ferromagnetism vs. Charge Ordering in the Pr <sub>0.5</sub> Ca <sub>0.5</sub> MnO <sub>3</sub> and La <sub>0.5</sub> Ca <sub>0.5</sub> MnO <sub>3</sub> Nanocrystals Phys. Rev. B 81(2) 024403 (2010)	Z. Jiráček, E. Hadová, O. Kaman et al.	50
Measurement of the Depth of Maximum of Extensive Air Showers above 10 <sup>18</sup> eV Phys. Rev. Lett. 104(9) 091101 (2010)	Pierre Auger Collaboration	281
Domain Walls of Ferroelectric BaTiO <sub>3</sub> within the Ginzburg-Landau-Devonshire Phenomenological Model Phys. Rev. B 81(14) 144125 (2010)	P. Márton, I. Rychetský, J. Hlinka	59
Adaptive Modulations of Martensites Phys. Rev. Lett. 104(14) 145702 (2010)	S. Kaufmann, U. K. Rossler, O. Heczko et al.	105
Anomalous Hall Effect Rev. Mod. Phys. 82(2) 1539–1592 (2010)	N. Nagaosa, J. Sinova, S. Onoda et al.	571
Influence of the Electron-cation Interaction on Electron Mobility in Dye-sensitized ZnO and TiO <sub>2</sub> Nanocrystals: A Study Using Ultrafast Terahertz Spectroscopy Phys. Rev. Lett. 104(19) 197401 (2010)	H. Němec, J. Rochford, O. Taratula et al.	63
First-principles Theory of Dilute Magnetic Semiconductors Rev. Mod. Phys. 82(2)1633–1690 (2010)	K. Sato, L. Bergqvist, J. Kudrnovský et al.	379
Brightly Luminescent Organically Capped Silicon Nanocrystals Fabricated at Room Temperature and Atmospheric Pressure ACS Nano 4(8) 4495–4504 (2010)	K. Kůsová, O. Cibulka, K. Dohnalová et al.	61

Title	Author(s)	Citations
A Multiferroic Material to Search for the Permanent Electric Dipole Moment of the Electron Nat. Mater. 9(8) 649–654 (2010)	K. Rushchanskii, S. Kamba, V. Goian et al.	35
A Strong Ferroelectric Ferromagnet Created by Means of Spin-Lattice Coupling Nature 466(7309) 954–U72 (2010)	J. H. Lee, I. Fang, E. Vlahos et al.	259
Systematic Study of Mn-doping Trends in Optical Properties of (Ga,Mn)As Phys. Rev. Lett. 105(22) 227201 (2010)	T. Jungwirth, P. Horodyská, N. Tesařová et al.	30
Spin Hall Effect Transistor Science 330(6012) 1801–1804 (2010)	J. Wunderlich, B. G. Park, A. C. Irvine et al.	81
Interplay of Conductance, Force, and Structural Change in Metallic Point Contacts Phys. Rev. Lett. 106(1) 016802 (2011)	M. Temes, C. Gonzalez, C. P. Lutz et al.	54
Applications of Quantum Monte Carlo Methods in Condensed Systems Rep. Prog. Phys. 74(2) 026502 (2011)	J. Kolorenč, L. Mitas	55
Forces and Currents in Carbon Nanostructures: Are We Imaging Atoms? Phys. Rev. Lett. 106(17) 176101 (2011)	M. Ondráček, P. Pou, V. Rozsival et al.	38
A Spin-Valve-Like Magnetoresistance of an Antiferromagnet-Based Tunnel Junction Nat. Mater. 10(5) 347–351 (2011)	B. G. Park, J. Wunderlich, X. Martí et al.	107
Composition Engineering in Cerium-Doped (Lu,Gd) <sub>3</sub> (Ga,Al) <sub>5</sub> O <sub>12</sub> Single Crystal Scintillators Crystal Growth & Design 11(10) 4484–4490 (2011)	K. Kamada, T. Endo, K. Tsutumi et al.	117

Title	Author(s)	Citations
Conical Defects in Higher Spin Theories J. High Energy Phys. 3(096) (2012)	A. Castro, R. Gopakumar, M. Gutperle et al.	41
Creation and Diagnosis of a Solid-Density Plasma with an X-ray Free-electron Laser Nature 482(7383) 59–U75 (2012)	S. M. Vinko, O. Ciricosta, B. I. Cho et al.	63
Spin Hall Effect Devices Nat. Mater. 11(5) 382–390 (2012)	T. Jungwirth, J. Wunderlich, K. Olejník	94
Direct Measurements of the Ionization Potential Depression in a Dense Plasma Phys. Rev. Lett. 109(6) 065002 (2012)	O. Ciricosta, S. M. Vinko, H.-K. Chung et al.	52
Observation of a New Particle in the Search for the Standard Model Higgs Boson with the ATLAS Detector at the LHC Phys. Lett. B 716(1) 1–29 (2012)	ATLAS Collaboration	2759
Evidence for the Spin-0 Nature of the Higgs Boson Using ATLAS Data Phys.Lett. B 726(1–3) 120–144 (2013)	ATLAS Collaboration	151
Crystallographic Computing System JANA2006: General Features Z. Kristallogr. 229(5) 345–352 (2014)	V. Petříček, M. Dušek, L. Palatinus	169
Room-Temperature Antiferromagnetic Memory Resistor Nat. Mater. 13(4) 367–374 (2014)	X. Martí, I. Fina, C. Frontera et al.	31

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