The 30th anniversary

ANNUAL REPORT

of the MTA SZFKI

2011

RESEARCH INSTITUTE FOR SOLID STATE PHYSICS AND OPTICS
Hungarian Academy of Sciences, Budapest, Hungary

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ANNUAL REPORT 2011

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We dedicate this volume to the memory of our former director János Kollár, who passed away on 11th January, 2011.

Dear Reader,

It is my pleasure to hand over the 18th edition of the Annual Report of the Research Institute for Solid State Physics and Optics. This is a special issue to commemorate the 30th anniversary of SZFKI. The institute was founded in 1981 as one of the institutions of the Hungarian Academy of Sciences. Its history though is rooted in the 1950s, when the Central Research Institute for Physics was established at Csillebérc at the same location. Some of our researchers had started their professional career at the former research establishment and made the first steps to initiate new research fields. Some of the topics were so forward looking that they are still relevant today.

Celebrating the jubilee, we share some personal memories of our first director. We offer a short overview of the most significant research results achieved during these fruitful decades. A representative list of the most relevant publications – papers, which have been cited over 100 times, or the ones that were published recently in high-ranking journals – is also included. Today following the footsteps of our charismatic predecessors – leaders and colleagues – we try to further strengthen the scientific reputation of our institute.

Currently, our staff of 201 includes 138 scientists. This year we have published over 283 papers in highly ranked international journals and conference proceedings showing a steadily high publication rate over recent years. Another volume of the textbook: "Fundamentals of Physics of Solids" by Jenő Sólyom was published.

In 2011 our institute started two important new projects. In the framework of the program "Momentum - From Brain Drain to Brain Gain" of the President of the Hungarian Academy of Sciences, Péter Domokos was among the 2011-year-winners. From our institute he is the second young scientist winning this grant. His research project is devoted to the quantum measurement theory in hybrid mesoscopic systems.

The other significant project coordinated by our institute is the grant entitled "Establishment of the Budapest Research Centre for ELI Laser Technology" within the framework of the New Széchenyi Program,. This is the next step forward after the preparatory phase of ELI, which has entered into the implementation stage. Professor Norbert Kroó and Aladár Czitrovszky were invited to be members of the ELI-ALPS Scientific Advisory Committee, which is one of the high priority scientific initiative of the European Community.

The achievements of our scientists have been acknowledged by several awards and nominations. Jenő Sólyom won the Széchenyi Prize, József Janszky received the Hungarian Republic, Officers's Cross Order of Merit and Péter Szépfalusy was awarded the Hungarian Order of Merit Cross with the Star. Róbert Szipőcs has received the Patent Excellence Award issued by the Hungarian Academy of Sciences and the National Patent

Office. This year Orsolya Kálmán received the Young Scientist Prize and Zoltán Donkó was given the Prize of Physics of the Hungarian Academy of Sciences. János Asbóth was awarded by the prestigious Junior Prima Award in Science category, for his outstanding achievements in quantum theory. The first director of our institute professor Norbert Kroó was awarded the Prima Primissima Prize (Hungarian Science). Ádám Gali obtained the degree of Doctor of Sciences at the Hungarian Academy of Sciences and 6 of our young researchers have received their PhD degrees.

It has become our tradition to deliver prizes for outstanding publication activity and applied research, respectively. In this year, two Publication Prizes were awarded to László Péter for his works on the properties of electrodeposited metals. Péter Hartmann received the prize for the investigation of collective phenomena in complex plasmas. The Applied Research Prize was shared by Péter Dombi and Péter Rácz for the development of long-cavity femtosecond laser oscillations.

I hope this booklet will provide you some useful information regarding the activities of the institute. The key figures offer a general overview of our Institute as a whole. In order to facilitate access to our scientists, we included their direct e-mail addresses in the Annual Report for your convenience. For further information please visit our homepage at http://www.szfki.hu.

In May 2011, the President of the Hungarian Academy of Sciences initiated the restructuring of the academic research network. According to this concept, our institute and the Research Institute of Nuclear and Particles Physics will form the Wigner Research Centre in the future.

We are looking forward to the new challenges.

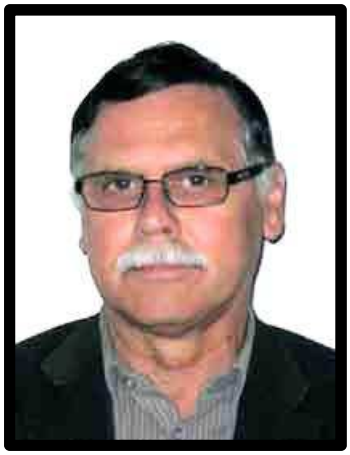
Budapest, December 5, 2011.

Ágnes Buka
Director

"Peace cannot be kept by force; it can only be achieved by understanding."

Albert Einstein

JÁNOS KOLLÁR
1945-2011



János Kollár acted as the director of our institute from 1998 to 2011; prior to this period, between 1989-1997 he was our deputy director. He started his scientific career here and remained faithful to this institute until the end of his life. He left university as a well-educated young physicist of extraordinary ability. His way of thinking was logical and objective as required of fresh graduates studying natural sciences. The physics of metals became the main focus of his interest. He gained an international reputation as a specialist of the theory of transition metals and was recognized as one of the leading experts of the surface properties of these materials. He was also a creative contributor to the density functional theory and its application to solid state physics.

János himself was a quiet and introverted person who expressed himself in brief to-the-point sentences. He was able to handle almost any situation with placid dignity, and when something disappointed him, only then, did he doubtingly shake his head or make a humorous remark. He was able to pass on this serenity to those around him; perhaps this was the reason that our institute was a peaceful environment, where he continuously ensured fairness, and strived to maintain balance between the various departments and groups.

As director he followed the path of his predecessor. The institute's remarkable results, acknowledged by both Hungarian and international surveys, were accomplished in a great part due to the tranquil atmosphere and strong working ethic he promoted through effective focus on research. His attitude followed from his personal character. He was able to address people with incredible tolerance, benevolence and wisdom. Everybody could expect from him a wise and insightful piece of advise. He helped his colleagues find their own scientific interest not only through his encouraging words, but also his supportive actions.

In addition to managing the institute, he catalyzed a wide range of scientific activities based upon his vast international connections. Until the very last minutes of his life he was working on research assignments together with his colleagues and PhD students, publishing articles on the characteristics of ferromagnetic transition metals, electronic charge density and anomalous relaxation. He kept offering an ever-increasing fraction of his time and effort to the benefit of the broader scientific community. He was elected president of the Eötvös Lóránd Physical Society, member of the ERA Committee of Engineering, and, in 2010, corresponding member of the Hungarian Academy of Sciences, acknowledging thereby not only his personal scientific achievements, but also his valuable contributions in the interest of scientific development in general.

All those who knew János Kollár appreciated him as an excellent physicist, an emphatic colleague and a wonderful person.

We will remember him with the greatest respect.

MY FEW THOUGHTS ON THE 30th ANNIVERSARY OF SZFKI

Solid state physics and optics research began on the Csillebérc Campus in the 1950's, shortly after the Central Research Institute for Physics of the Hungarian Academy of Sciences has been found. The Institute underwent extensive restructuring throughout the decades, a process which is still ongoing. 1975 was the first year in which researchers at the campus working in related fields formed a distinct organizational structure, which later came to be known as the Institute of Solid State Research (SZTKI). At the time SZTKI did not function as an independent legal entity within the Central Research Institute for Physics (KFKI), but as a unit comprised of several departments within the broader framework of KFKI. The Institute initially consisted of three departments working in solid state physics, as well as one in the field of optics, complemented by a technical support group. A further restructuring in 1981 combined these five groups into the current Institute. A scientific director was appointed at the Institute, although still not an independent legal entity, with the mission to foster basic research and innovation in the fields of solid state physics and optics. I was personally involved in the early creation of the legally independent institute. First I was a scientific director of the SZTKI until 1992, then following further restructuring I became the director of the newly formed Research Institute for Solid State Physics (SZFKI) between 1992-1998.

The creation of the new independent institute was by no means a simple task. Some colleagues expressed worries not only regarding the future of solid state physics and optics research, but also voiced concerns about personal failures on my part. Fortunately, the majority of researchers were optimistic about our future and cherished our common objective of creating a successful research organization.

Soon after the SZFKI was founded, a world known French physicist accepted our invitation to visit our institution. During our conversation before his departure, he spoke of a French custom; if French scientists are invited and the visit is funded by the host institution, the custom is that the scientists summarize in writing their impressions and experiences of their visit for the benefit of the host institution. Thus our French colleague felt obliged to share his opinion with us. He told us that an institute like ours – the SZFKI – must be the world leader in at least one speciality and he pinpointed some topics in the field of solid state physics and optics in which we satisfy these criteria. I was of course very happy with his appraisal and I tried to do my best - by all possible means – to safeguard our high quality standards of these distinguished special topics. Our guest also shared with me his critical remarks. His outside perspective and evaluation were of utmost importance in the challenging task of evaluating topics of study, and deciding how to allocate support between topics.

To my great pleasure, throughout the lifetime of the Institute, decisions concerning critical issues were always preceded by serious panel discussions and debates, even after my term as the director. Such discussions of course did not lighten the personal liability of the leader. I benefited greatly from such brainstorming sessions, especially during the difficult transition period of the early 1990's when funding became scarce and being able to reach a consensus on critical issues, as well as being able to identify with issues facing the Institute became of utmost importance.

Later, the steadily increasing number of research grant opportunities, together with the introduction of value-based evaluation systems combined increased the effectivity of our research teams. Thanks to these factors SZFKI came to be ranked as one of the top

research institutes within the Hungarian Academy of Sciences, as well as according to international standards.

As the primary source of funding of the Institute comes through taxpayer revenues, I felt obliged to utilize our capabilities in ways reaching beyond our scientific endeavors. I expected my colleagues to partake in advancing higher education through teaching courses as they found appropriate. As a result of such collaborative efforts with higher education, a satellite faculty of ELTE University was given home on our campus. In addition we placed great emphasis on the sharing of our research results, facilities, equipment and methodologies with the greater scientific and economic community.

It came as a great relief to me that the management of the Institute stayed in good hands, even after my leave while taking government office, and subsequently during my participation in the leadership of the Hungarian Academy of Sciences beginning in 1998. My successor headed the institute with dignity in the same spirit. It has become the painful and unfortunate reality that I can no longer thank my late successor in person for his past efforts.

Norbert Kroó

SHORT HISTORY AND SURVEY OF THE MOST RELEVANT RESULTS OF THE SZFKI

The establishment of the Research Institute for Solid State Physics and Optics (SZFKI) of the Hungarian Academy of Sciences (HAS) can be dated back to 1981 when the "Research Institute for Solid State Physics" was formed within the Central Research Institute for Physics (KFKI, founded in 1950) of HAS. By the end of 1991, the research centre KFKI was decentralized and SZFKI became one of the successor institutes and also an independent legal entity of HAS. In 1981, as a result of a further consolidation of the research network of HAS in 1998, the Research Laboratory of Crystal Physics (established in 1976), part of the Research Laboratory of Natural Sciences of HAS until then, was merged with SZFKI. As a consequence the name of the institute has also changed to "Research Institute for Solid State Physics and Optics of the HAS".

The mission of the institute is nevertheless unchanged, conducting basic research in the fields of theoretical and experimental solid-state physics and materials science. Areas actively investigated include metal physics, crystal physics, liquid crystal research as well as theoretical and experimental optics (laser physics, quantum optics, and the interaction of light with matter). Our experimental research rests on a broad variety of techniques including x-ray diffraction, NMR, Mössbauer and optical spectroscopy. We conduct neutron scattering experiments at the Budapest Neutron Centre, a large-scale on-campus research facility. Our application oriented research and development program focuses on optical thin films, applications of laser technology, growing of optical crystals, and metallurgy.

Looking back to the thirty years of SZFKI research, it is inevitable to summarize the most important results. Thousands of scientific publications – part of them published together with researchers of other national and foreign establishments – attest the effectiveness; and some of the most significant achievements are mentioned here. A national network of research infrastructures was established primarily in the fields of nuclear methods (neutron, NMR, Mössbauer spectroscopy), X-ray studies, laser development and applications, magnetic and dielectric measurements. New technologies were implemented for growing optical crystals, preparing thin films and multilayers as well as amorphous and nanocrystalline alloys. Internationally quoted theoretical schools were formed in the fields of solid state physics, statistical physics, and optics. A survey performed by ICSU (International Committee of Science Unions) in 1993, deemed the work of the institute "especially efficient".

SZFKI has got vivid and close relationships in all of its research areas with a great number of European and overseas universities and research institutes. This is well demonstrated by having at least one foreign co-author in most of their publications. The important forms of our international relations are short-term bilateral visits, long-term foreign work, hosting visiting scientists and students and participation in joint research projects. Since 1992, the institute participates in the EU Framework Programs (FP) with a variety of projects. In 2000, SZFKI became Center of Excellence, as the host institute of a consortium on Condensed Matter in four academic institutes. Recently the institute participated in the preparatory phase of three European mega-projects (X-ray Free Electron Laser - pre-XFEL, the Extreme Light Infrastructure - ELI-PP, and the European Spallation Source - ESS). The institute completed several national (OTKA, OMFB, government financed development projects) and other international projects (EUREKA, COST, NATO Science for Peace projects, etc.), too.

The co-workers of the SZFKI are active in the education of solid state physics, optics, material science and chemistry in several universities, (Eötvös University (ELTE), Budapest, the Budapest University of Technology and Economics (BME), Universities of Szeged (SZTE) and Pécs (PTE), the Semmelweis University, Budapest (SOTE)). This is realized in giving regular and special lectures, supervising laboratory practices, diploma works and PhD students. Researchers of the SZFKI contributed to the enhancement of the level of education by writing numerous textbooks, and book chapters. Since 1989, a Physical Education Laboratory of ELTE operates in the SZFKI. The measurements available in this laboratory became part of the regular laboratory practices for students in physics. Further, elevated-level practices are also available that extend to more serious examinations. It is the special research infrastructure of the institute (special material samples, liquid He, high magnetic field, availability of unique research facilities, e.g. laser technique, etc.) which makes possible these measurements.

At present, the organizational scheme of SZFKI contains 10 scientific departments (Theoretical Solid State Physics; Experimental Solid State Physics; Complex Fluids; Metals Research; Neutron Physics; Neutron Spectroscopy; Laser Physics; Laser Applications; Crystal Physics; Quantum Optics and Quantum Information). The Campus Library serving all the KFKI successor institutes is also part of SZFKI.

It is not an easy task to summarize shortly the most important results of the past thirty year activity of the institute. In the following, each department highlights its contribution, then a list of selected publications is given.

Department of Theoretical Solid State Physics

The most interesting discoveries in solid state physics of the 1960s, 1970s and 1980s, namely the Kondo effect, low-dimensional organic conductors, valence fluctuating and heavy-fermion materials, and high-temperature superconductivity, made a lasting impact on the research topics of the solid state theory department. They were in the forefront of research carried out during the last thirty years. The works related to the Kondo effect found a natural continuation in the study of the low-temperature properties of metallic glasses, the behaviour of two-level systems interacting with a degenerate electron gas, and the dissipative motion of heavy particles in fermion systems. The description of the ground state of mixed-valence and heavy-fermion metals based on the variational solution of the periodic Anderson model was another natural extension. Some of these works are highlighted in the book Lecture Notes on Electron Correlations and Magnetism by Patrik Fazekas.

The anomalous properties of low-dimensional organic conductors were studied in two different ways. On the one hand, the renormalization group method was used to describe the behaviour, the eventual instabilities of the quasi-one-dimensional Fermi gas. On the other hand, role of impurities were clarified in the charge- and spin-density wave state. The d-wave state found in unconventional spin-density wave systems is already related to high-temperature superconductivity. We could also interpret the Raman spectra of high Tc materials, nanotubes, graphene and amorphous metals.

In the 1980s, the department was actively engaged in the field of classical and quantum chaos, in the description of nonlinear dynamical systems, and in quantum optics, especially in the interaction of intense electromagnetic radiation with matter.

Besides these topics, several coworkers of the department were involved in the study of phase transitions in classical and quantum systems, the role of frustration, and the properties of amorphous systems and spin glasses. The algorithmic developments of the

density-matrix renormalization group allowed not only a more detailed study of the ground state of spin-chain and spin-ladder models, but found applications in quantum-chemistry problems. We found new types of excitations in exactly solvable one-dimensional models using the Bethe ansatz, and determined the finite-size corrections.

A team studied the electronic states of metals, especially the surface states and the magnetic properties of surfaces. The collected data base is the most reliable in the field.

Teaching activity was always strength at the department. Our professors gave regular courses for graduate students, mostly at ELTE. The main achievement of this teaching activity is the three-volume book on Fundamentals of the Physics of Solids written by Jenő Sólyom. The English translation of this work is a widely used textbook at different universities.

Department of Experimental Solid State Physics

In the last 30 years, the study of materials at the forefront of international research with up-to-date methods was in the focus of the department and its predecessors. In cooperation with the worldwide research community we studied metallic glasses, one-dimensional organic conductors and charge-density wave materials, high temperature superconductors, fullerenes and carbon nanotubes by transport, magnetic and spectroscopic methods. Our specific experimental strengths include X-ray diffraction and holography, Mössbauer spectroscopy, infrared and optical spectroscopy.

The local atomic structure of metallic glasses was determined by Mössbauer spectroscopy to be similar to that of the metastable compound formed during the crystallization process. A method was proposed which resulted in the discovery of formerly unknown metastable crystalline phases and supported an internationally accepted, trigonal prism-based amorphous alloy model.

In a diffraction experiment the phases of the scattered radiation are lost which is a serious hindrance, since the unmeasured phases carry more information on the crystal structure than the measured amplitudes. To recover the phases and thus determine crystal structures, we have developed a mathematical technique, called charge flipping. The algorithm is based on sparseness, a rather weak assumption on the electron density. It also works in a truly ab initio manner – no information on atoms, chemical composition or symmetry is utilized. Besides its theoretical relevance, the charge flipping method is increasingly applied in practice; successful examples are ranging from single crystals to powders, from periodic to aperiodic structures, from complete small-molecule arrangements to protein heavy-atom substructures.

In holography, unlike in diffraction, phases of the scattered radiation are also measured by recording an interference pattern with a reference beam. The theory of atomic resolution hard x-ray holography was developed. Later we also demonstrated experimentally the viability of the method on several materials using the fluorescent radiation of an atom as the reference beam. This work was highlighted in well known scientific and general public media.

In 1991, we started the studies of fullerenes, the molecular allotropes of carbon. Our field of research included the preparation, structure and physical properties of crystalline derivatives of these spherical molecules. Our most significant results were the recognition of the polymeric nature of the fulleride ions in some alkali metal salts of C_{60}, and the determination of the crystalline structures of a series of related materials. This work initiated intensive studies on the polymerized fullerenes. A further important result was the

discovery of a new family of cocrystals, the rotor-stator phases of fullerenes and cubanes. These crystals consist of rotating fullerene balls surrounded by the molecular bearings of static cubanes. The spectacular prototype of this family, $C_{60}{\cdot}C_8H_8$, is the unique representative of the highest possible symmetry cocrystals.

We studied extensively the optical properties of transparent carbon nanotube networks in the frequency range from the far infrared through the ultraviolet. We used high-quality single-walled carbon nanotube samples from the best sources available and discovered several effects in several frequency ranges. In the terahertz region, we found the presence of an electronic gap due to curvature of the nanotubes, in the infrared, dipole-active vibrational modes of the tubes, and in the near infrared and visible, selectivity of chemical reactions involving the sidewalls. These properties have significant consequences in the applications of these materials as transparent conductors, replacing the rare, expensive and toxic indium tin oxide layers.

A coarse-grained field theoretical model has been developed for describing polycrystalline self-organization, which captures for the first time the formation of such complex solidification morphologies as disordered dendrites, crystal sheaves, spherulites, and fractal-like polycrystalline aggregates. This result made for the cover page of Nature Materials, and the editorial board of Science News (USA) has selected it as the 15th most important result in all branches of physics in 2004.

Department of Complex Fluids

Our research group was established in 1972 to investigate physical properties of and phenomena characteristic for liquid crystals. The initial aims were demonstration of electro-optic effects usable for display applications, study of phase transitions and miscibility of liquid crystals, and exploring molecular dynamics by neutron and dielectric spectroscopy. The latter soon became the most powerful tool of the laboratory which resulted in pioneering results on dielectric relaxation in nematic and various smectic phases. Besides those, experimental proofs for two, chirality induced cross effects in cholesterics, the thermomechanical and the diffusio-mechanical couplings, mark the end of our first decade.

In the middle of the 80s the research fields have completely been renewed. For a decade the ferroelectric chiral smectic C* liquid crystals have got into the focus; their linear electromechanical effect has been discovered and understood first by our group. In parallel two new research directions have been initiated: light-induced effects and pattern formation in liquid crystals; both still form a major part of our present activities. The nonlinear optical investigations initially aimed at the optical bistability as well as at the optical reorientation first of pure, later of dyed nematics. The latter phenomenon, the dye-induced shift of the threshold of optical reorientation is now called Jánossy-effect after its discoverer and interpreter (our colleague). At present these activities mainly transformed into studies of the interactions between liquid crystals and polymeric and/or light activated surfaces. In the field of pattern formation, surface and bulk instabilities have been addressed as well. Regarding the first type, our coworkers have obtained pioneering results on viscous fingering of nematics and smectics, as well as on the mesophase growth at a first order phase transition (an analog to crystallization). As far as bulk instabilities are concerned, our group has contributed to the experimental studies and theoretical understanding of flow induced patterns, to field induced nonlinear transient patterns and to electroconvection. In electroconvection, which is in the focus of our present activities even now, due to a 20 years long powerful collaboration with theoreticians at the Bayreuth University, our group is regarded as prominent experts of the field.

In the new millennium, besides the two continued research lines, new topics have attracted attention. Following the international trends, investigation of banana shaped liquid crystals has been started. The discovery of giant flexoelectricity in our new banana nematic compound is one of our latest outstanding results. Recently we also realized that flexoelectricity plays a vital role in pattern formation as well, therefore at present this phenomenon became an important current target of our research. In the last decade, we expanded our scope from simple liquid crystals also to more complex fluids, like liquid crystalline polymers/elastomers, liquid crystal composites (nematics doped with nanoparticles), and granular materials. The latter topic required establishing new experimental methods (e.g., high-speed digital imaging) which allows studying dynamics of dry and wet granular materials of various type and shape.

The research of physical properties of complex fluids has been supported and supplemented from the beginning by an organic synthetic chemistry laboratory. Compounds provided by our chemists had a vital importance whenever the main target of research was modified and samples were not yet available commercially or via co-operations. By now a huge number of new molecules have been synthesized in our lab; many of them have been supplied to collaborating research groups all over the world.

During these decades our group has gained a good international reputation in the field of complex fluids. As an indication of that we have three times got the opportunity to organize large international conferences (in 1979, 1994 and 1997).

Department of Metals Research

The Metals Research Department was established in 1972. The first few years were devoted to theoretical studies of phase transformations in metals and alloys, experimental investigations of dilute impurities in Cu, Fe and Al by NMR, Mössbauer and electrical transport and specific heat measurements as well as to an industry-oriented research programme into the decarburization of iron and the internal oxidation of copper.

A rapid-quenching technology from the melt (so-called melt-spinning) was introduced to produce these metastable materials (e.g., Fe-B alloys) and the existing electrodeposition method was also adapted for this purpose (e.g., Ni-P alloys). A flourishing research on the preparation and the study of thermal stability, magnetic and transport properties, atomic and electronic structure of a large variety of metallic glasses has developed. Soft magnetic amorphous alloys were in the forefront of this activity in view of prospective applications and several patents were filed in this field. In the SEM laboratory, a stroboscopic method was developed for observing static and dynamic domain patterns in ferromagnetic metals and alloys by using back-scattered electrons.

Research was started on amorphous alloy hydrogen systems (e.g., Zr-Ni-H) in 1985 which activity lasted over two decades and was directed mainly towards H diffusion studies by NMR and to H-induced phase separation. Currently, the focus of rapid quenching and ball milling technology is the investigation of bulk amorphous and nano-crystalline alloys.

In the early 1990s, research was carried out on electrodeposited nanocrystalline metals (mainly Ni) for a few years and some papers from this work have become frequently cited in this still active area. In the mid nineties, an activity was started in wide international collaboration on the electrodeposition of magnetic/non-magnetic multilayers exhibiting the GMR effect. Important contributions to this field which were summarized in an extended review paper published in Progr. Mater. Sci. in 2010 include the clarification of the underlying electrochemical processes controlling layer formation, the introduction of an unconventional deposition pulse sequence (galvanostatic/potetiostatic pulse combination)

and revealing the microstructure and the role of superparamagnetic regions in these multilayers. There has been recently also work by applying the secondary neutral mass spectroscopy in external collaboration to unravelling in-depth compositional profiles in electrodeposited thin films and multilayers.

Several department members participated in research on high-Tc superconductivity by NMR and several important papers were published on the vortex behaviour in these materials. There was an activity also on CDW and SDW materials by NMR and quantum Hall effect measurements. The study of low-dimensional materials has been recently extended to graphene as well.

The NMR group has been involved for a long time in the study of biological materials in collaboration with members of domestic medical universities. This includes, among others, the study of cataracta in various eye lenses in the late 1970s. In recent years, the structurally disordered proteins are in the focus which work is carried out together with the Institute of Enzymology of HAS and it has already led to well-acknowledged results about clarifying the hydration behaviour of these materials.

Since 2008, a geologist joined the department and established here the study of various rock minerals for a clarification of the evolution of the lithosphere and interactions between different geospheres. The study of rocks plays an important role in the understanding of slow chemical reactions in solid phase material, since the duration of laboratory experiments is limited. Our research interest is focused on the mechanisms and kinetics of micro-structure evolution and the development of sub-micron-sized chemical heterogeneities during chemical reactions between solid phases.

There has been an activity in the department also on developing various non-destructive measurement techniques, a digital lock-in amplifier and a hydrogen permeation measurement facility.

Department of Neutron Physics and Spectroscopy

Application of neutrons in the solid state research has long traditions in Hungary; the home base for this activity is the Budapest Research Reactor (BRR) which was first started in 1959 and is situated on the KFKI site.. The establishment of SZFKI in 1992 coincides with the restart of BRR after a major reconstruction. This 10 MW multi-purpose reactor became a unique large-scale facility in the Central European region and that time the Hungarian Academy of Sciences decided to open reactor facilities to the international user community. SZFKI took the lead on the organisation of this user research activity in the field of neutron scattering for condensed matter, materials science, engineering research by using and constructing spectrometers at the horizontal channels of the reactor. Also in 1992 the Budapest Neutron Centre (BNC) – a consortium of neutron based laboratories with other institutes at the KFKI site – was established with major contribution from SZFKI.

Thanks to the expanding international collaborations the SZFKI neutron team was one of the first in the country to receive an EU grant under the project WENNET (West-East Neutron Network). This project allowed us to start extending the instrument capacity at BRR from the initial 4 instruments to 15 experimental stations by now (8 of them belong to SZFKI). We make part of the Neutron Muon Integrated Infrastructure Initiative (NMI3) project in EU FP5, FP6 and FP7. This project gathers the 10 major European neutron source facilities, including BNC to provide access and research opportunities for a wide community of researchers. In 2008 resuming the previous 4 years activity, the international community has highly appreciated the BNC contribution: at the concluding general

assembly meeting 4 European experts presented in different fields a selection of highlights out of the nearly 1000 experiments performed in the frame of NMI3. In 2009 another FP7 project was started, we have been invited as the "neutron facility" in the CHARISMA projects, which puts together a consortium of large European museums (Louvre, British Museum, Prado…) and scientific facilities to join efforts for the investigation of objects of cultural heritage.

A few important milestones should be mentioned: a liquid hydrogen cold source was installed and the neutron guide system was replaced by a supermirror guide configuration, yielding a factor of 50-80 gain in neutron intensity. In 2002-2004 a second guide hall was constructed to house a new time-of-flight instrument.. SZFKI is one of the centres of the development and applications of the so called Reverse Monte Carlo (RMC) simulation method of structural data evaluation. We have organised 3 international conferences over the past 10 years that were devoted to the various aspects of the RMC technique. One of the most important discoveries in neutron science of recent years is neutron holography. Our team has developed the concept and realised experimentally the 3D holographic imaging of structures at atomic level resolution by the use of neutron interference. We devote considerable effort to education and training of young researcher and newcomers to the field. In 2010 the first comprehensive neutron scattering textbook was published in Hungarian. Our Central European Training School (CETS) – lectures by renowned scientist and hands-on training at our facilities during a week – has now 12 years traditions and it has become very popular.

Department of Laser Physics

The project "Interactions of Intense Laser Fields with Matter", as a straightforward continuation of the former decades' activities, performed experimental and theoretical studies of interactions of intense short laser pulses with metal surfaces, atoms and free electrons aiming to demonstrate fundamental QED processes. Increasing the laser intensity from low to extreme high values, the group revealed first in the literature a number of new effects: from the perturbative (multiphoton) to the nonperturbative (optical tunnel) basic phenomena, creating possibilities for the realization, of new type, e.g., very short electron and X-ray pulses. As a result, it was this group where the worldwide first published proposal for the generation of attosecond (1 as = 10^{-18} s) pulses came from in the year 1992 giving birth to attosecond science. The group has been involved in the theory of attosecond phenomena ever since. The theoretical study of light-matter interaction formulated a laser induced double layer model to interpret several of the project's previous experimental results. Beyond semiclassical methods, the quantal phase-space properties of electromagnetic radiation, photon correlations, and gauge-invariant Wigner distributions have also been analyzed in various contexts. The theory of nonlinear processes in strong laser fields and the experimental investigation of ultra-fast processes with femtosecond lasers as well as femtosecond photonics developments represent recent research directions. Researchers of the group recently demonstrated the generation of few-cycle surface plasmon wavepackets for the first time as well as the existence of strong-field photoemission and photo-acceleration processes in surface plasmon fields.

In the "Laser Physics" project basic research has been conducted for many years on several types of gas lasers and also in related fields, especially in spectroscopy (line width and line broadening studies). The gas laser research has started with the near infrared (1.15 nm) He-Ne laser, and ended with the deep ultraviolet (224 nm) He–Ag ion laser, which has the shortest wavelength among the continuous wave lasers ever operated, providing unique possibilities in laser Raman spectroscopy. Different novel high-voltage hollow

cathode discharge arrangements were developed and have been applied as pumping sources of noble gas mixture and metal ion lasers.

Motivated by the interest in the pumping medium, the experimental investigation and computational simulation of gas discharges has grown as a new direction of research. The electrolyte cathode atmospheric glow discharge (ELCAD) for direct analysis of heavy metal content of solutions was worked out. A thorough investigation of its operation mechanism and processes determining the emitted intensities have been carried out. Other glow discharges for biomedical purposes have been studied and their elementary reactions have been characterized.

Computer simulation codes based on fluid and kinetic approaches have been developed to describe basic phenomena and processes in glow discharges. Successful research on multidimensional lasers and on multispectral ellipsometry has been accomplished. Studies of complex (strongly-coupled) plasmas represent a more recent line of research as well. Molecular dynamics simulation codes have been developed, which made it possible to characterize static and thermodynamic properties, as well as collective excitations and wave propagation in these systems. Most recently two experimental apparatus have been built up for the investigations of (i) complex (dusty) plasmas and (ii) asymmetric charge transfer processes (playing important role in plasma chemistry).

In the field of "Metal Optics" pioneering work was carried out related to surface plasmon polaritons including their fundamental investigation, propagation properties and decay. According to our recent (experimental and) theoretical results, the light emitted by single surface plasmons shows a transition from anti-bunching to bunching of the photon counting events in a Hanbury Brown – Twiss type apparatus. In addition, optical investigation of fullerene films was performed, and the optical behavior of hydrogenated Pd films was studied. Also, a multichannel spectrometer was constructed, and a near-field optical study of grainy noble metal films was carried out.

Department of Laser Applications

Laser applications have a long tradition in our institute. In the seventies, the focus was put on the practical use in materials processing and special medical application. Later the interest shifted from the application in measurement technique to the development of laser particle counters and sizers in the eighties, to application in environmental protection and high-tech fields such as the clean room monitoring. In 2000's, a new measuring instrument (Dual Wavelength Optical Particle Spectrometer – DWOPS) was developed for simultaneous sizing, counting and estimation of the complex refractive index of aerosol particles in the sub-micron and micron size-range.

For the environmental monitoring of atmospheric aerosols and measurement of air contamination a micro-bus was equipped with a mobile laboratory for environmental measurements. Using different instruments we measured the atmospheric aerosols and toxic gases in different location during different seasons of the year. Measurements were carried out in several districts within the city of Budapest and its surrounding, in the Ferihegy Airport and several industrial locations. The collected data were compared with the statistics of the adverse health effects to the pregnancy where significant negative influence was determined. The aerosol particle deposition in human respiratory tracks was modelled and specific deposition parameters were also studied.

Furthermore the activity of the department was widened to the development of new techniques and methods for studying photon statistics, generation of non-classical squeezed light, investigation of plasmon statistics, etc.

Remarkable results were achieved, like the elaboration of new standardless method of the measurement of absolute quantum efficiency of the photodetectors using entangled photon pairs, development of the single-photon source with pre-programmable number of photons, high time resolution statistical data evaluation system for measurement of the time distribution and correlation function of photons generated in different non-linear processes. Investigation of the properties of the excitation light and the light emitted by surface plasmons showed the similarity of these statistics at low light intensities.

In the last years, one of the main activities of the department was the participation in EU ESFRI Project within the 7th Framework Program, Extreme Light Infrastructure – Preparatory Phase. In the project 13 countries were involved. ELI ERIC would be the first large infrastructure dedicated to the fundamental study of laser-matter interaction in a new and unsurpassed regime of laser intensity: the ultra-relativistic regime (IL>1023 W/cm²). The participation of the Hungarian side was coordinated by our institute. As a result of the successful preparatory phase, the Attosecond Infrastructure facility - ALPS will be built in Szeged, Hungary.

Already in the beginning of nineties a fruitful cooperation was started with the Technical University of Vienna for the research and development of optical coatings useful in ultrafast laser applications. We have made an important contribution to the ultrafast laser technology with inventing and producing of the first chirped mirrors for compensation the positive dispersion in Ti:sapphire lasers in the year 1994. Working together with the Vienna Group and a Group in Groningen (in the Netherlands) we were decreased the world record of the laser pulse length close to 4 fs. Based on our common scientific results in the field of femtosecond lasers a new ultrafast laser technology has been developed, providing a strong basis for the economic utilization of above results in the form of small size private enterprises. These spin-off enterprises were established in the right time, and have reached a significant market share and have been manufactured many thousands of of special mirrors and optical elements for femtosecond Ti:sapphire lasers for the world scientific community.

The Amorphous Semiconductor research group was working in the field of a-Si:H thin films in the ’80s. They made solar cells having 15% efficiency based on this material. In the ‘90s amorphous carbons were in the focus of research. New ways were found to control the optical, electronic and surface characteristics of these materials. The advantageous properties of amorphous carbon nanoparticles and thin films were exploited in supercapacitors and protective coatings for medical devices developed for Hungarian companies as end-users in cooperation with international partners. Starting from mid-2000s increased attention was given to nanodiamonds. Grain boundaries, surface modification and formation of color centers are the main directions of the research aiming to find new ways for application of these nanomaterials. New methods were worked out to identify the surface groups and to form stable color centers in nanodiamonds.

Department of Crystal Physics and Technology

After joining the SZFKI in 1998, the Crystal Physics Department resumed its activities in the growth and study of non-linear optical and scintillator crystals, including both basic and applied research. Investigation and modification of the crystal’s real structure to obtain improved physical properties for applications, and discovery of new phenomena have been in the focus of the research.

The study of the phase relations in the K_2O-Li_2O-Nb_2O_5 system lead us to the growth of ferroelectric stoichiometric $LiNbO_3$ (sLN) and $K_3Li_2Nb_5O_{15}$ (KLN) crystals with tailored

physical properties. Based on UV-VIS-IR absorption spectroscopy, Raman scattering and dielectric measurements, quantum chemical defect models have been developed to interpret the compositional changes and the presence of hydroxyl ions. Trapping of charges leading to polaron-type or impurity related centers has been characterized by various time-resolved optical and paramagnetic resonance methods. Among the most promising results is Mg-doped sLN with suppressed photorefractive damage suitable for application in high energy terahertz pulse generation.

Borates are widely used e.g. for higher harmonic generation of laser light. We have developed various growth techniques for the preparation of beta-BaB_2O_4 (BBO), LiB_3O_5 (LBO), $Li_2B_4O_7$ (LTB), $CsLiB_6O_{10}$ (CLBO), $YAl_3(BO_3)_4$ (YAB), $GdAl_3(BO_3)_4$ (GAB), $Li_6Y(BO_3)_3$ (LYB) and $Li_6Gd(BO_3)_3$ (LGB). Efficient chemical etching techniques, optical and electron microscopic methods were developed to reveal growth defects. Hydroxyl ions in as-grown LBO, LTB, YAB and water molecules in CLBO have been observed by FTIR spectroscopy. Luminescence characteristics and energy transfers in tissue-equivalent LTB:Cu:Ag dosimeters and several double-doped YAB crystals were described using high resolution optical spectroscopic methods; the term schemes of some involved rare-earth ions in YAB were also determined by crystal field calculations.

Beside niobates and borates numerous other oxide crystals have also been studied. In sillenites, systematic trends were discovered for the symmetrical and asymmetrical vibrational modes of the impurity-centered oxygen octahedra as a function of atomic mass and impurity charge. Diffractive optical elements and waveguides were designed and fabricated by ion implantation in optical crystals and also in tellurite glass and silica. Self-fixed, page-oriented digital holograms were written by continuous and *ns* pulsed laser exposure into photorefractive Bi_2TeO_5.

Recent demand on new materials in optical and radiation detection technologies points towards nanocrystals prepared by different wet chemical methods. Accordingly, nanopowders e. g. embedded in various matrices represent a new direction in materials engineering also for the Crystal Physics Department.

Department of Nonlinear and Quantum Optics

Quantum optical treatment of nonlinear optical processes was the key for further development of laser physics, at the end of the 1980s, to prosperous new directions. Jozsef Janszky has launched research along this line and had significant contribution to the understanding of noise processes at the ultimate quantum level, to the creation and characterization of the non-classical states of light in terms of coherent-state representations of the radiation field. This work has diversified in the mid-90s with the involvement of several students. For example, the theoretical details of quantum state reconstruction have been worked out, supporting the successful experimental realizations in several leading laboratories around the world.

The research spectrum of the Department of Quantum Optics and Quantum Information was vastly enlarged with the young researchers defining and conducting their own projects and became a true center on the international quantum optics landscape. Several (altogether 8) international topical scientific conferences were organized by the department, creating a possibility to actively participate in the progress of the field and meet the members of the scientific community.

Rapid experimental progress in quantum optics raised hopes about the utilization of the far reaching consequences of coherent quantum dynamics combined with suppressed noise and high precision detection in the 1990s. The new field of quantum information theory

has been born in these years and grew then very fast. We participated in this progress from the beginning with a number of results covering several aspects, ranging from the theory of quantum teleportation to the analysis of quantum walks.

As a natural extension of nonlinear optical processes with quantized fields, we have studied coherent control mechanisms in molecular and atomic systems. We have worked out several adiabatic control schemes for controlling the atomic states. One of the main achievements of this work is a robust qubit rotation scheme. In cooperation with the Crystal Physics Department, we have developed an experimental laboratory to study resonant nonlinear optical processes in doped inorganic crystals grown in house.

A substantial part of recent and current research of the department focuses on cavity quantum electrodynamics, which is one of the most important quantum optical systems devoted to the study of light-matter interaction at a fundamental microscopic level of single atoms and single photons. In recent years, we achieved influential results in the theoretical description of ultracold atoms within a high-finesse cavity, which stimulated experimental effort and led ultimately to the first observation of a Dicke-type quantum phase transition.

Another fundamental aspect of light matter interaction is the understanding of the electronic properties of atoms and molecules. Spectroscopy and vibrational spectroscopy in particular, is one of the main techniques for discovering the structure and dynamics of molecular species. The analysis of complicated vibrational spectra often calls for theoretical modeling based on high level ab initio electronic structure calculation and methods suitable for solving the Schroedinger equation of a Hamiltonian of several variables and strongly anharmonic potential energy surface.

We have contributed to the development of a currently state-of-the-art method, the so called discrete variable representation method, solving the vibrational Schroedinger equation. Applications of this method however are not restricted to the Schroedinger equation and it has been employed to solving various equations in mathematical physics, for example the Fokker-Planck equation.

Publications

This is the list of the most significant publications of the coworkers of the Research Institute for Solid State Physics and Optics, published partly in the ancestor institutes. This list includes selected publications with citations higher than 100. The more recent important publications that appeared in high impact factor journals are given separately.

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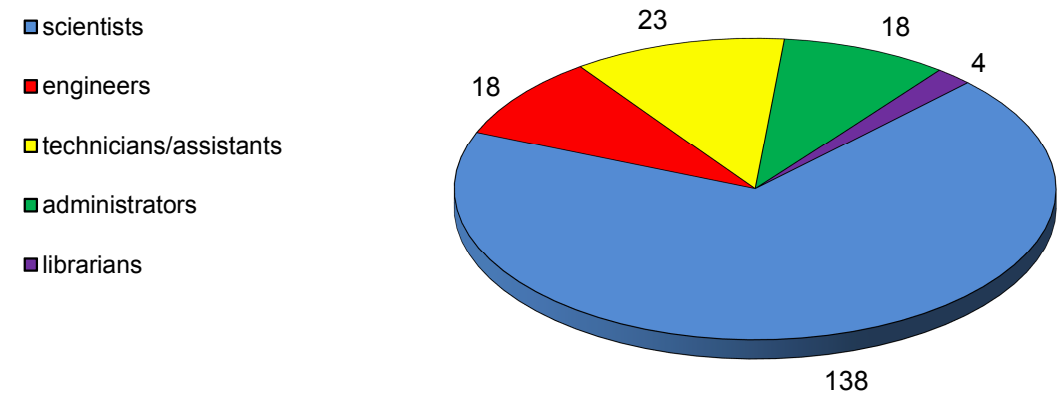
KEY FIGURES

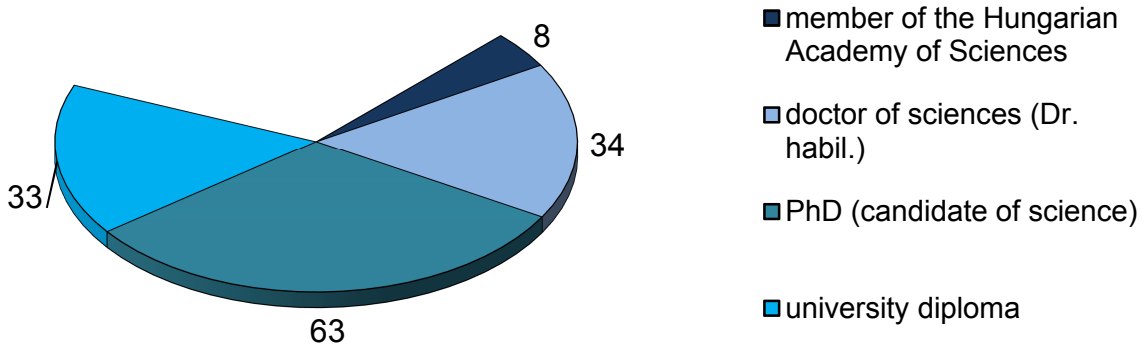
Permanent staff of the institute: 201 employees.

Its **distribution by professions**:

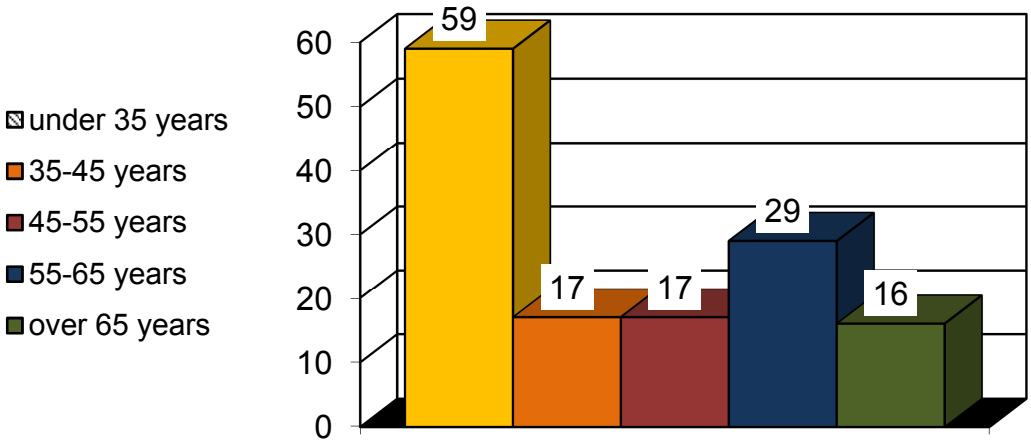


Distribution of scientists:

a) by scientific titles/degrees:

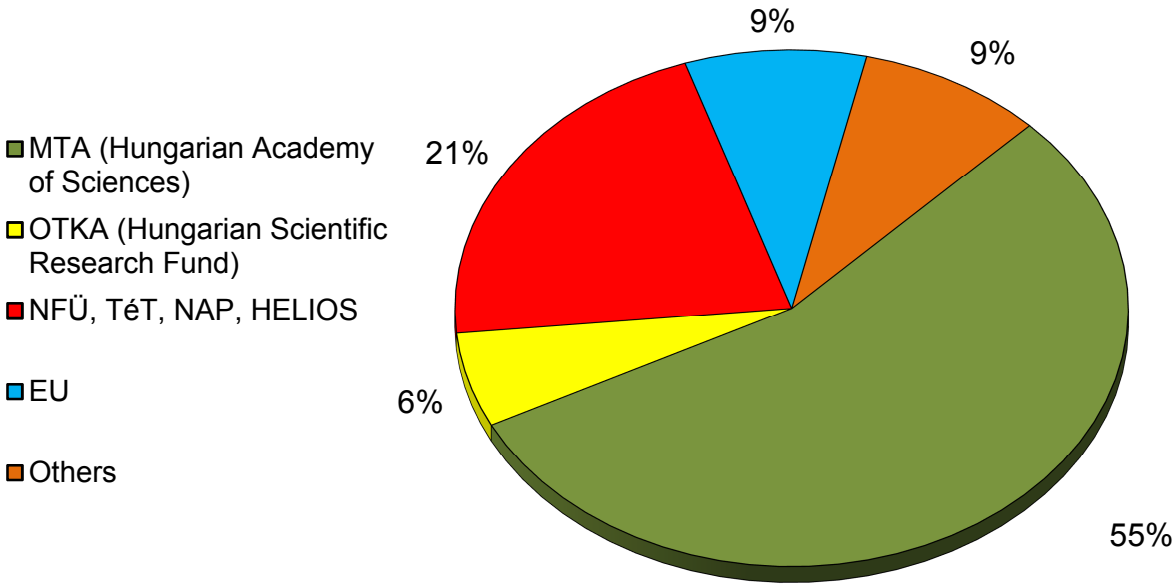


b) by age groups:

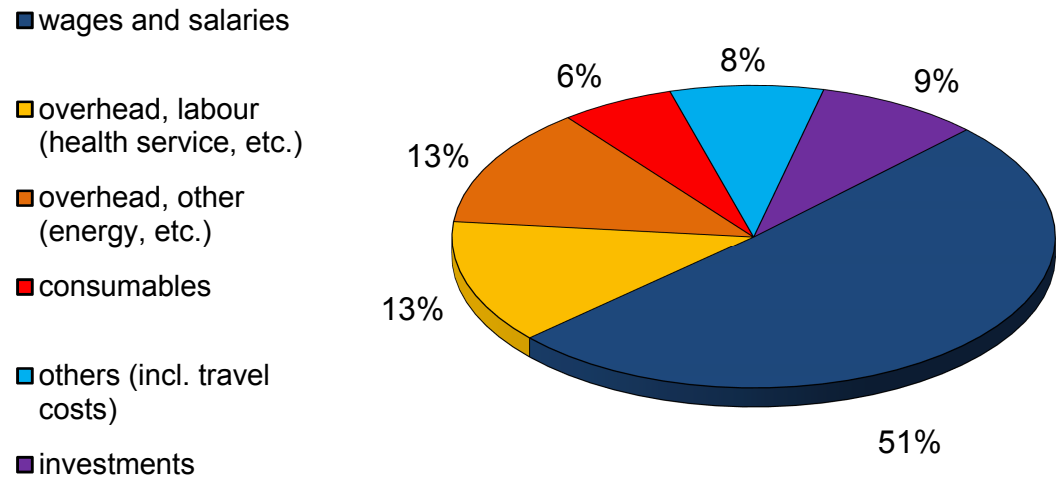


Financial management

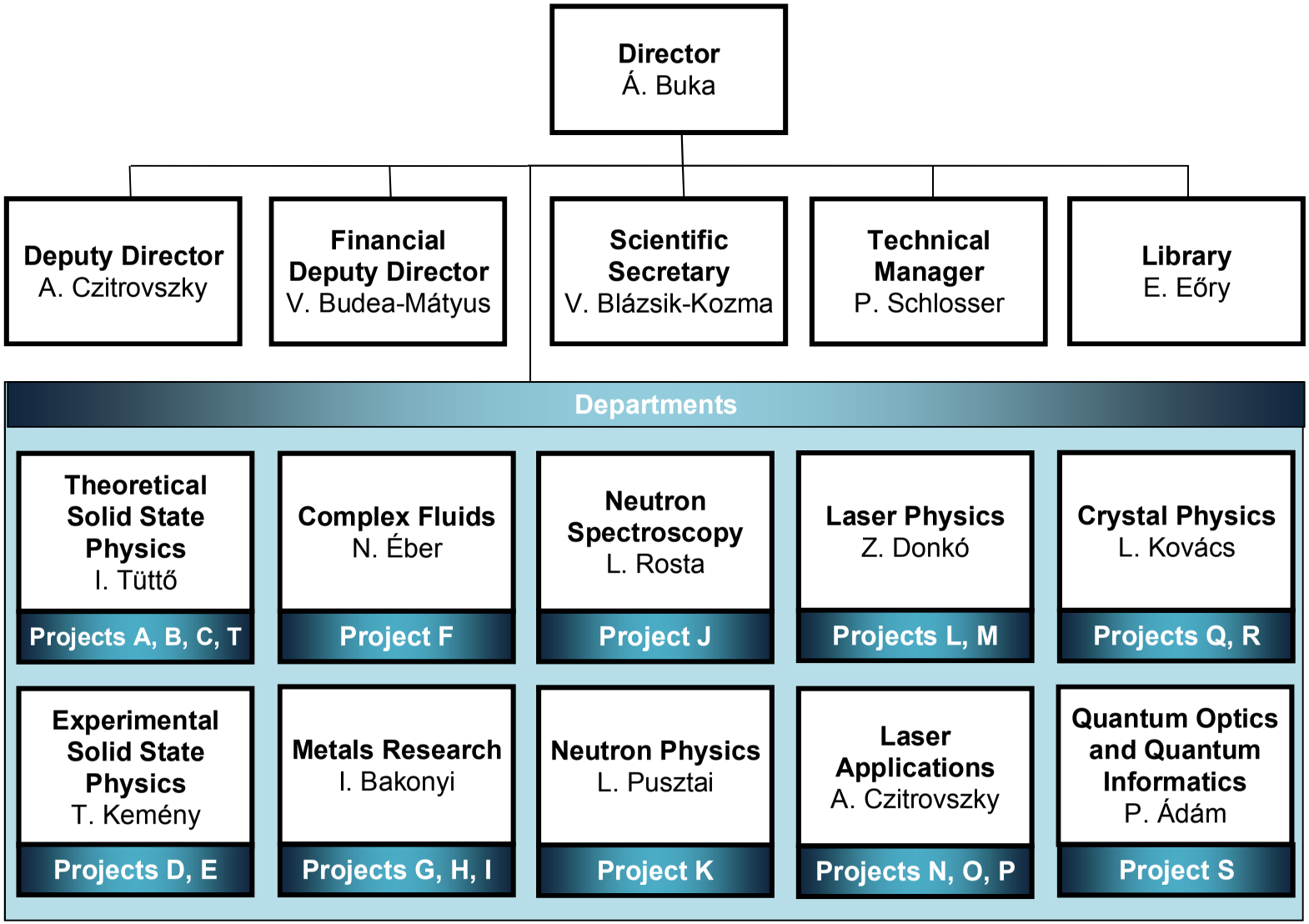
a) Sources of operation costs:



b) Distribution of expenditures:



Structural diagram of the Research Institute for Solid State Physics and Optics



A. STRONGLY CORRELATED SYSTEMS

J. Sólyom, G. Barcza[#], I. Hagymási[#], A. Kiss, M. Lajkó[#], Ö. Legeza, K. Penc, J. Romhányi[#], L. Seabra[+], E. Szirmai, K. Vladár, F. Woynarovich

Anderson and Kondo problem. — Strongly correlated electron systems are in the forefront of present-day physics due to both fundamentally open issues and the application of such systems in modern electronics or spintronics. However, unravelling the fundamental phenomena and successful applications require further studies which can only be performed by advanced numerical techniques. The recently developed continuous-time quantum Monte Carlo (CT-QMC) simulation method is a very powerful numerical technique to investigate dynamic and magnetic properties of correlated electron systems. It significantly advances the limit of conventional quantum Monte Carlo methods, and opens new perspectives in a wide range of physical problems. Using the CT-QMC method, we have investigated Kondo impurity systems with potential scattering and orbital degeneracy in a wide temperature range across the Kondo temperature. We have derived accurate numerical results for static and dynamic physical quantities. It has been shown in the limit of strong potential scattering that (i) the resistivity decreases with decreasing temperature in contrast to the ordinary Kondo effect; (ii) the quasiparticle density of states obtains the antiresonance around the Fermi level; (iii) thermopower and thermal conductivity also show anomalous behaviour. Furthermore the magnetic susceptibility follows the universal temperature dependence for any values of the potential scattering. We pointed out that strong potential scattering may have relevance in real systems. For example, recent STM experiments have found that the density of states shows antiresonance in the normal phase of URu_2Si_2, and the resistivity decreases with decreasing temperature in the dilute system $U_xTh_{1-x}Ru_2Si_2$.

We have performed detailed analysis of an extended periodic Anderson model, where the interaction between conduction electrons is also taken into account. We used a variational method and exact diagonalization to attack the problem. It has been shown that the interaction significantly shifts the energy range of f-orbitals, where heavy-fermion behaviour might be observed.

Exotic magnetic orders of high-spin ultracold atoms. — The search for new quantum phases of matter, one of the main themes in the field of electronic materials with strong correlations, has become an important aspect of the physics of cold atoms, too. A recent development concerns the possibility of loading multi-color fermions in optical lattices, which has renewed the interest in the SU(N) Heisenberg model that describes the permutation of N-color objects on a lattice. In condensed matter, these models require fine tuning of the parameters. By contrast, the simple quantum permutation embodied by the SU(N) Heisenberg model is a realistic starting point to describe the Mott phase of N-color fermions at filling 1/N (one fermion per site). While it is intuitively clear that Mott insulating states will exist at particular commensurate fillings, the nature and spatial structure of multi-flavor Mott insulating states are in general not well understood. For example, on the square lattice geometry, many different proposals for insulating states have been put forward, ranging from SU(N) symmetry breaking ”magnetic” states to dimerized or plaquette states, chiral spin liquids and staggered flux phases. Combining a semi-classical analysis, exact diagonalizations, and a variational approach based on a

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tensor network ansatz (infinite projected entangled pair states, iPEPS), we have studied the problem on the square lattice. We have shown that the Mott insulating state of three-flavor (N=3) fermions develops a stripe-like three-sublattice long-range order in the strong-coupling limit. This surprising pattern for a bipartite lattice with only nearest-neighbour interactions is shown to be the consequence of a subtle quantum order-by-disorder mechanism. Even more interestingly, for the SU(4) case we show that both spatial and SU(4) symmetries are simultaneously broken: the ground state is spontaneously dimerized, and on each strong dimer, two colors dominate and combine into a 6-dimensional irreducible representation of SU(4). In the resulting pattern, the same color does not appear on neighbouring dimers, so that if two colors are dominant on one dimer, nearest-neighbour dimers are dominated by the remaining two colors, resulting in a Néel-like arrangement.

We have suggested a novel method to analyze the magnetic properties of higher-spin ultracold atoms loaded into an optical lattice within the concept of site and bond spin. The treatment is based on mapping the strongly repulsive fermion models with on-site interaction to one with nearest-neighbour interaction, and making a convenient rearrangement of the interaction terms exploiting their symmetry properties. We have shown that similar mapping can be applied for boson systems, too. Applying this treatment to spin-3/2 fermions on a two-dimensional square lattice at quarter filling, the mean-field equations were analyzed for repulsive singlet g_0 and quintet g_2 couplings. We found that the realization of the U(1) plaquette state predicted in other works for the special couplings $g_0 = g_2$ does not require such a fine tuning, it is stable in an extended region of the phase diagram. This phase competes with an SU(2) plaquette state. In both cases the U(1) and SU(2) flux, respectively, passing through the plaquettes labels the different gauge-non-equivalent states. We have investigated the influence of external magnetic field on the SU(2) flux state and have found that it becomes the ground state of the system in the presence of weak applied magnetic fields.

For spin-5/2 fermion system at 1/6-filling the parameter space is three dimensional. We have shown that in the plane, where the multiparticle interaction can be neglected, the ground state is either antiferromagnetic or an U(1) plaquette phase with zero flux.

We have studied the SU(6) symmetric model of strongly repulsive spin-5/2 fermions on a honeycomb lattice. We have found that the ground state of the system is a chiral spin-liquid state with $2\pi/3$ flux per plaquette, which spontaneously violates time-reversal invariance. We have demonstrated that due to the breaking of time-reversal symmetry, the system exhibits quantum Hall effect and chiral edge states. We have also shown how the experimentally accessible spin fluctuations relate to the emerging gauge field dynamics. We have shown that the lowest energy competing order has a staggered flux like order analogously to the π-flux state of spin-1/2 fermions on a square lattice and the next-lowest order is a valence bond crystal with disconnected elementary plaquettes.

Frustrated magnetic systems. — We have revisited the phase diagram of the frustrated s=1/2 spin ladder with antiferromagnetic rung and diagonal couplings. In particular, we have reexamined the evidence for the columnar dimer phase, which has been predicted from analytic treatment of the model and has been claimed to be found in numerical calculations. By considering longer chains and by keeping more states than in previous works using the DMRG method, we have shown that the numerical evidence presented previously for the existence of the dimerized phase is not compelling.

$ZnCr_2O_4$ is a prototypical example of highly frustrated magnets. Despite strong antiferromagnetic exchange interactions between neighbouring Cr ions, $ZnCr_2O_4$ fails to order magnetically down to a very low temperature that is just a few percent of the temperature anticipated from mean field theory. The unconventional nature of magnetism in $ZnCr_2O_4$ raises the possibility that it might also exhibit new forms of order in magnetic field. Indeed, it has been known for long that the interplay between magnetic field and frustrated exchange interactions can lead to both a magnetization plateau, i.e., magnetic "solids" which break the translational symmetries of the lattice, and spin-flopped phases, i.e., magnetic "superfluids" with well-defined magnetic order in the plane perpendicular to the magnetic field. One particularly intriguing proposal is that magnetic field might stabilize phases which break both sets of symmetries simultaneously. Such a phase would be a magnetic analogue of the "supersolid" long sought in ^4He. For a long time, testing these predictions for materials like $ZnCr_2O_4$ was rendered impossible by the need for multiple extremes: magnetic fields in excess of 100 T and temperatures of a few kelvin. Now, a new generation of pulsed high-field magnets and advances in instrumentation at the Institute of Solid State Physics of the Tokyo University made it possible to explore this physics for the first time. We have reported the first determination of the magnetic phase diagram of $ZnCr_2O_4$, through Faraday rotation, for magnetic fields of up to 190 T, and temperatures down to 4.2 K. We found evidence for three distinct magnetic phase transitions, the 1/2 magnetization plateau, a 3:1 canted phase, and a 2:1:1 canted phase, all of which were predicted and are well-described by a simple model based on spin-lattice coupling that was developed by us. These results provide a beautiful illustration of the phenomenon of "order by distortion", the subtle interplay between spin and lattice degrees of freedom in a frustrated magnet.

Completely integrable system. — Recently we have shown that the O(1) corrections due to the saddle point fluctuations to the macroscopic free energy of Bethe Ansatz systems is obtained correctly if the precise definition of the partition function in terms of the quantum numbers is used. A refinement of these calculations led to a more detailed understanding of the question of nontrivial normalization of the partition function.

Quantum-chemical applications of the DMRG algorithm. — We have studied transition metal clusters, i.e., two isomers of Cu_2O_2, from a quantum information theory perspective using the density-matrix renormalization group (DMRG) method. Our results indicate the importance of taking entanglement among molecular orbitals into account in order to devise an optimal orbital ordering and to carry out efficient calculations for open d-shell systems. We have proposed a recipe to perform DMRG calculations in a black-box fashion and we point out the connections of our work to other tensor network state approaches.

We have continued our study of the elementary excitations of a Hamiltonian model for the π-electrons in poly-diacetylene chains including electron-phonon interactions as well. We have shown that inclusion of lattice relaxation is mandatory in order to determine the energy spectrum and to reproduce experimental values.

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OTKA K73455 Quantum phases and phase transitions in tunable correlated systems (K. Penc, 2008-2012)

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Long term visitor

— L. Seabra, postdoctoral position for 6 months, now in MPIPKS Dresden

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B. COMPLEX SYSTEMS

F. Iglói, R. Juhász, I. Kovács, A. Sütő, P. Szépfalusy

The principal interest of this group is the theoretical investigation of different aspects of equilibrium and non-equilibrium statistical physics and quantum systems.

Phase transitions and critical behaviour. — We have studied magnetic friction between two systems of q-state Potts spins which are moving along their boundaries with a relative constant velocity v. Due to interaction between the surface spins there is a permanent energy flow and the system is in a steady state which is far from equilibrium. The problem has been treated analytically in the limit $v=\infty$ (in one dimension, as well as in two dimensions for large-q values) and for v and q finite by Monte Carlo simulations in two dimensions. Exotic nonequilibrium phase transitions are found to take place, the properties of which depend on the type of phase transition in equilibrium. When this latter transition is of first order, a sequence of second- and first-order nonequilibrium transitions has been observed when the interaction is varied.

We have developed a very efficient numerical algorithm of the strong disorder renormalization group method to study the critical behaviour of the random transverse-field Ising model, which is a prototype of random quantum magnets. With this algorithm we can renormalize an N-site cluster within a time $N \log N$, independently of the topology of the graph and we went up to $N \sim 4\text{x}10^6$. We have studied regular lattices with dimension $D \leq 4$ as well as Erdős-Rényi random graphs, which are infinite dimensional objects. In all cases the quantum critical behaviour is found to be controlled by an infinite disorder fixed point, in which disorder plays a dominant role over quantum fluctuations. As a consequence the renormalization procedure as well as the obtained critical properties are asymptotically exact for large systems. We have also studied Griffiths singularities in the paramagnetic and the ferromagnetic phases and generalized the numerical algorithm for another random quantum systems.

We studied the prototype of driven diffusive systems, the asymmetric simple exclusion process in the presence of random-force disorder within the mean field approximation. We calculated the stationary current through a domain with reversed bias and found that the results are in agreement with earlier intuitive assumptions. A phenomenological random barrier model has been applied in order to describe quantitatively the coarsening phenomena. Predictions of the theory were compared with numerical results obtained by integrating the mean field evolution equations. The results suggest that the less complex mean field model belongs to the same universality class as the original stochastic model does.

We proved that weak limits as the density tends to infinity of classical ground states of integrable pair potentials minimize the mean-field energy functional. By studying the latter we derived global properties of high-density ground state configurations in bounded domains and in infinite space. Our main result is a theorem stating that for interactions having a strictly positive Fourier transform the distribution of particles tends to be uniform as the density increases, while high-density ground states show some pattern if the Fourier transform is partially negative. The latter confirms the conclusion of earlier studies by Vlasov (1945), Kirzhnits and Nepomnyashchii (1971), and Likos *et al.* (2007). Other results include the proof that there is no Bravais lattice among high-density ground states of interactions whose Fourier transform has a negative part and the potential diverges or has a cusp at zero. For a class of nonnegative, range-1 pair potentials in one dimensional

continuous space we proved that any classical ground state of lower density ≥1 is a tower-lattice, i.e., a lattice formed by towers of particles the heights of which can differ only by one, and the lattice constant is 1. The potential may be flat or may have a cusp at the origin, it can be continuous, but its derivative has a jump at 1. The result is valid on finite intervals or rings of integer length and on the whole line.

Quantum systems. — We have developed a quantitative semi-classical theory for the non-equilibrium dynamics of transverse Ising chains after quantum quenches, in particular sudden changes of the transverse field strength. We have obtained accurate predictions for the quench dependent relaxation times and correlation lengths, and also about the recurrence times and quasi-periodicity of time dependent correlations in finite systems with open or periodic boundary conditions. We have compared the quantitative predictions of our semi-classical theory (local magnetization, equal time bulk-bulk and surface-to-bulk correlations, and bulk autocorrelations) with the results from exact free fermion calculations and discuss the range of applicability of the semi-classical theory and possible generalizations and extensions.

We have extended the pseudopotential theory to the Bogoliubov-De Gennes equations to determine the excess energy when one atom is added to the trapped superfluid Fermi system with even number of atoms. Particular attention has been payed to systems being at the Feshbach resonance point. The results for relatively small particle numbers are in harmony with the Monte-Carlo calculations, but are also relevant for systems with larger particle numbers. Concerning the additional one quasiparticle state we have defined and determined two new universal numbers to characterize its widths.

3-fluid hydrodynamic equations have been formulated for a spin-1 Bose gas in the presence of a magnetic field. The modes (first sound, second sound, quadrupolar spin wave) have been calculated for different values of the coupling constants. In particular the hybridization between the second sound and the spin wave modes have been studied. It has been pointed out that the quadrupolar spin wave plays the role of the critical mode, when the system goes over to the phase, where a 2-fluid hydrodynamics is valid, by changing the temperature and/or the magnetic field.

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OTKA T075324	Effects of disorder in many body systems (F. Iglói, 2009-2012)
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Publications

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See also: E.22.

C. ELECTRONIC STATES IN SOLIDS

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Density functional calculations. — Due to the increased electron density within the surface layer, metal surfaces are generally expected to have tensile surface stress. Using first-principles density functional calculations, we demonstrated that in magnetic 3d metals surface magnetism can alter this commonly accepted picture. We find that thermodynamically stable surfaces of chromium and manganese possess compressive surface stress. The revealed negative surface stress is shown to be ascribed to the enhanced magnetic moments within the surface layer relative to bulk values.

A metallic solid solution or glassy mixture, consisting of components which are immiscible at low temperature, is thermodynamically unstable when quenched from high temperature and phase separation occurs during aging or annealing. The phase separation may take place through two different paths: nucleation and growth and spinodal decomposition. For both paths, the interfacial energy between the decomposed phases plays an important role. The interfacial energies (g) between the Cr-rich a'-Fe_xCr_{1-x} and Fe-rich a-$Fe_{1-y}Cr_y$ phases ($0<x$, $y<0.35$) were calculated to be between ~0.02 and ~0.33 Jm^{-2} for the ferromagnetic state and between ~0.02 and ~0.27 Jm^{-2} for the paramagnetic state. Although for both magnetic states, the interfacial energy follows a general decreasing trend with increasing x and y, the fine structures of the $g(x, y)$ maps exhibit a marked magnetic state dependence. The subtleties were shown to be ascribed to the magnetic interaction between the Fe and Cr atoms near the interface. We also showed that the interfacial energies and the interfacial energy anisotropy are highly composition dependent. In particular, the increasing interfacial energy anisotropy with decreasing compositional gap may induce different morphology of the decomposed phases for different compositions of the host alloys.

We compared the performances of three common gradient-level exchange–correlation functionals for metallic bulk, surface and vacancy systems. We found that approximations which, by construction, give similar results for the jellium surface, show large deviations for realistic systems. The particular charge density and density gradient dependence of the exchange–correlation energy densities are shown to be the reason behind the obtained differences. Our findings confirm that both the global (total energy) and the local (energy density) behaviour of the exchange–correlation functional should be monitored for a consistent functional design.

The stacking fault energy is a parameter of significant importance on the mechanical properties of close-packed face centered cubic alloys, such as strength, toughness and fracture. The alloying effects of Mn, Co and Nb on the stacking fault energy (SFE) of austenitic stainless steels, Fe–Cr–Ni with various Ni contents, were investigated via quantum–mechanical first-principles calculations. In the studied composition range, it is found that Mn always decreases the SFE at 0 K but increases it at room temperature in high-Ni alloys. The SFE always decreases with increasing Co content. Niobium increases the SFE significantly in low-Ni alloys; however, this effect is strongly diminished in high-Ni alloys. The SFE-enhancing effect of Ni usually observed in Fe–Cr–Ni alloys is inverted to an SFE-decreasing effect by Nb. The revealed nonlinear composition dependencies were explained in terms of the peculiar magnetic contributions to the total SFE.

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The phase stability of the 6*d* transition metals (elements 103–111) were investigated using first-principles electronic-structure calculations. Comparison with lighter transition metals reveals that the structural sequence trend is broken at the end of the 6*d* series. To account for this anomalous behaviour, the effect of relativity on the lattice stability was scrutinized, taking different approximations into consideration. It was found that the mass-velocity and Darwin terms give important contributions to the electronic structure, leading to changes in the interstitial charge density and thus, in the structural energy difference.

By using density-functional theory in combination with the coherent-potential approximation and the disordered local magnetic moment picture, we demonstrated that the competing high-temperature cubic phases of paramagnetic Fe correspond to two distinct total energy minima in the tetragonal (Bain) configurational space. Both the face-centered cubic (fcc) and the body-centered cubic (bcc) lattices are dynamically stable, and at static conditions the fcc structure is found to be the thermodynamically stable phase. The theoretical bcc and fcc bulk parameters are in agreement with the experimental data. Due to the shallow energy minimum around the bcc structure, increasing temperature is predicted to stabilize the bcc (δ) phase against the fcc (γ) one, in line with the phase diagram of Fe.

Stainless steel is a good example of a metal that is not easily machined. To explain such behaviour an understanding of the fundamental **adhesion** between the workpiece and the tool is invaluable. It is a well-known fact that build-up layers form in the interface, but little attention has been given to the very first layer that adheres to the tool surface. Although this layer rapidly becomes covered by successive material transfer, this layer and its ability to stick to the tool surface control the successive material transfer and influence the cutting properties. We employed a quick stop test to interrupt the cutting of a 316L stainless steel using a TiN-coated cemented carbide cutting insert. We used different analytical techniques, such as transmission electron microscopy, X-ray photoelectron spectroscopy and scanning electron microscopy, as well as theoretical atomistic modeling, to study the early adhesion.

EMTO. — Using density functional theory formulated within the framework of the exact muffin-tin orbitals (EMTO) method, we investigated the thermo-physical properties of bcc iron–magnesium alloys, containing 5 and 10 atomic % Mg, under extreme conditions, at high pressure and high temperature. The temperature effect was taken into account via the Fermi–Dirac distribution of the electrons. We found that at high pressures pure bcc iron is dynamically unstable at any temperature, having a negative tetragonal shear modulus (C'). Magnesium alloying significantly increases C' of Fe, and bcc Fe–Mg alloys become dynamically stable at high temperature. We discussed the electronic structure origin of the stabilization effect of Mg in detail. We showed that the thermo-physical properties of a bcc Fe–Mg alloy with 5% Mg agree well with those of the Earth's inner core as provided by seismic observations.

We investigated the elastic properties of body-centered cubic $Fe_{0.85}Ni_{0.1}Mg_{0.05}$ alloy at the conditions of the Earth's inner core, using the EMTO method. We demonstrated that in this system, the chemical stabilization effect of Mg is significantly larger than that of Ni. We showed that the elastic properties of $Fe_{0.85}Ni_{0.1}Mg_{0.05}$ are in good agreement with those of the Earth's inner core, as given by seismic observations. We found that the excellent mechanical properties of $Fe_{0.85}Ni_{0.1}Mg_{0.05}$ are primarily due to Mg.

We studied the exchange interaction in metals and on metal surfaces using first principles fully relativistic SKKR calculations. We found a typical 2D behaviour in the asymptotic regime where a surface state is present, and an exponentially decaying one when there is

none. We also studied the properties of the surface state, especially the higher order, non-symmetric Rashba-Bychkov effect in Bi/Ag(100) surface alloy. Based on relativistic first principles calculations we demonstrated that the splitting of the Bi sp_z surface band can not be satisfactorily described in terms of first order, isotropic Rashba Hamiltonian. Morover, we showed that the third-order term is subject to a large anisotropy, consistent with the dispersion relation deduced from our symmetry analysis. We also derived explicit formulas using **kp** perturbation theory for the third order anisotropy parameters, and established that the isotropic and anisotropic contributions are related to normal-to-plane and in-plane gradients of the potential respectively. Comparing the energy separation of the relevant orbital projected bands for Au(111) and Bi/Ag(111), the expressions can provide a qualitative understanding of the different nature of the Rashba-Bychkov splitting in these two systems.

Using the so called spin-cluster expansion, which is based on a relativistic first-principles electronic structure calculation, we obtained tensorial exchange parameters of a Heisenberg Hamiltonian in a Fe/Ir(100) thin film. Then it was used in a spin-dynamics simulation to obtain the magnetic ground state. In good agreement with experiments we found that up to 3 monolayers of Fe, there is no net magnetization in the system, while 4 monolayers and higher are strongly magnetic.

Metallic glass. — The Raman response of the metallic glass $Ni_{67}Zr_{33}$ is measured as a function of polarization and temperature and analyzed theoretically. Unexpectedly, the intensity in the range up to 300 cm^{-1} increases upon cooling, which is counterintuitive when the response originates from vibrations alone as in insulators. The increase finds a natural explanation if the conduction electrons are assumed to scatter on localized vibrations with a scattering probability proportional to the Debye-Waller factor. None of our assumptions is material specific, and the results are expected to be relevant for disordered systems in general.

Friedel oscillation in grapheme. — We investigate the local density of states and Friedel oscillation in graphene around a well-localized impurity in Born approximation. In our analytical calculations Green's function technique has been used taking into account both the localized atomic wave functions in a tight-binding scheme and the corresponding symmetries of the lattice. As a result we obtained long wavelength oscillations in the density of electrons with long-range behaviour proportional to the inverse square of the distance from the impurity. These leading oscillations are out of phase on nearby lattice sites (in fact for an extended defect they cancel each other within one unit cell), therefore a probe with resolution worse than a few unit cells will experience only the next to leading inverse cube decay of density oscillations even for a short-range scatterer.

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Grants and international cooperations

OTKA K68312 Complex analysis of magnetic nanostructure for high density recording (B. Újfalussy, 2007-2011)

OTKA K84078	Magnetic, mechanical and thermal properties of alloys and their surfaces (B. Újfalussy, 2011-2015)
STINT	Swedish-Hungarian joint project, Atomic-scale investigation of steel materials by first principles method (L. Vitos, 2009-2014)

Publications

Articles

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C.42. Vitos L, Zhang* H, Al-Zoubi* N, Lu* S, Nilsson* JO, Hertzman* S, Nilson* G, Johansson* B; Stainless steel alloys from first-principles theory; In: *7th European Stainless Steel Conference: Science and Market, 21-23 September 2011, Como Italy*; 2011

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C.43. Vitos L, Zhang* HL, Lu* S, Al-Zoubi* N, Johansson* B, Nurmi* E, Ropo* M, Punkkinen* MPJ, Kokko* K; First-principles quantum mechanical approach to stainless steel alloys; In: *Alloy Steel: Properties and Use*; InTech, ISBN 978-953-307-888-5, pp. , 2011.

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D. NON-EQUILIBRIUM ALLOYS

I. Vincze, J. Balogh, L. Bujdosó, D. Kaptás, T. Kemény, L.F. Kiss

Investigation of carbon nanotubes filled with ferrocene. — Carbon nanotubes have an interesting property: they can encapsulate other molecules in their "one" dimensional cavity. Iron containing organometallic molecules have very interesting electronic, magnetic and catalytic properties – their encapsulation into nanotubes seems to be rewarding. Double-walled carbon nanotubes can be created from nanotubes filled with metallocenes by annealing.

The most stable metallocene is the ferrocene $Fe(C_5H_5)_2$ which is well suited for Mössbauer investigations. It has stable and metastable forms having different crystal structures: at low temperatures the stable ferrocene is orthorhombic and above 242 K it is monoclinic. The monoclinic phase can be undercooled: below 242 K it becomes metastable and below 164 K it transforms to a metastable triclinic phase. The Debye temperatures of different crystal structures are different and relatively low (lower than room temperature). The normalized relative area in the Mössbauer spectra is proportional to the probability of the Mössbauer effect (the so-called f-factor), its temperature dependence is determined by the Debye temperature (θ_D). Temperature dependence of the normalized relative area for the different crystal structures is shown in Fig. 1. Using high temperature limit of the Debye model for the "f-factor", we get θ_D=128 K for the orthorhombic and θ_D=122 K for the metastable triclinic phase.

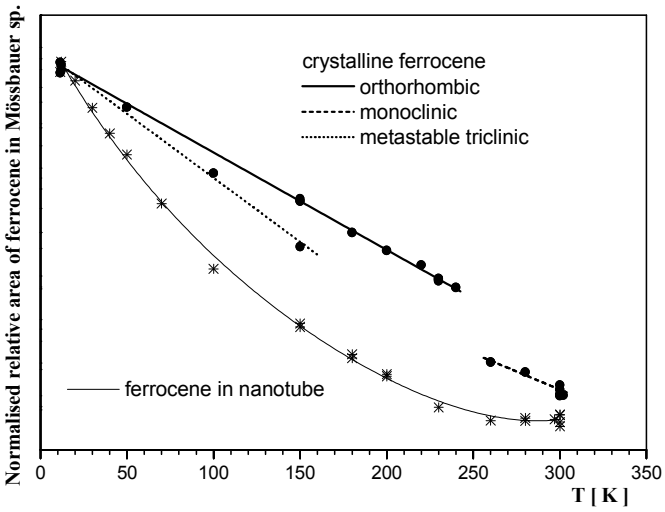

Fig. 1. *Normalized relative area of the ferrocene in the Mössbauer spectra as a function of temperature. This is proportional to the "f-factor" (probability of the Mössbauer effect) which depends on the Debye temperature of the sample. Dots show data measured on crystalline ferrocene; stars show data measured on ferrocene-filled carbon nanotubes. Lines are guides to the eye and indicate the different crystal structures of crystalline ferrocene*

In cooperation with research topic "E" we investigated a (P2 type) carbon nanotube sample filled with ferrocene. The single-walled nanotubes prepared by arc discharge were purchased from Carbon Solutions Inc. The average diameter of the nanotubes was 1.4 nm. The vapor method was used to fill the nanotubes with ferrocene molecules. The adsorbed ferrocene molecules were removed from outside of the nanotubes by washing the sample with ethanol and acetone.

The low temperature Mössbauer spectrum can be seen in Fig. 2. It shows that during the filling procedure some ferrocene molecules were decomposed producing cementite (Fe_3C) and iron-oxide. The Mössbauer parameters of the ferrocene molecules in the carbon nanotubes were the same as those of pure crystalline ferrocene. No charge transfer was detected between the delocalized electrons of ferrocene molecules and the inner wall of the

carbon nanotubes. Using the high temperature limit of the Debye model for the "f-factor", we get the Debye temperature of the ferrocene inside the nanotube as θ_D=76 K. This low value shows that the ferrocene clusters inside the nanotubes do not form bulk crystals and interact with the wall of the nanotube rather weakly. The significantly lower θ_D compared to the bulk crystalline values could be explained by the small size of the encapsulated clusters.

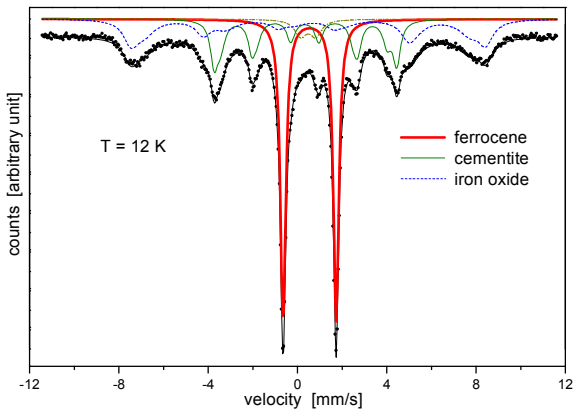

Fig. 2. *Mössbauer spectrum of single wall carbon nanotube filled with ferrocene.*

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Grants and cooperations

OTKA K68612 Magnetic anisotropy of structures with reduced dimension (L.F. Kiss, 2007-2011)

Publications

Articles

D.1. Kiss LF, Franco* V, Csontos* M, Péter L, Conde* CF, Conde* A, Kemény T, Tóth J, Varga LK, Bakonyi I; Analysis of the magnetoresistance contributions in a nanocrystallized Cr-doped FINEMET alloy; *J Magn Magn Mater*; **323**, 699-707, 2011

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See also: C.35., E.17.

E. X-RAY DIFFRACTION

G. Faigel, G. Bortel, N. Chelwani[#], L. Gránásy, Z. Jurek, K. Kamarás, G. Klupp, D. Kocsis[#], É. Kováts, K. Németh[#], G. Oszlányi, Á. Pekker[#], S. Pekker, T. Pusztai, Z. Szekrényes[#], Gy. Tegze[#], M. Tegze, H.M. Tóháti[#], Gy. Tóth[#]

Carbon based systems. — Lately various carbon based materials became the center of intensive research. Among them we studied fullerenes and related compounds, carbon nanotubes and graphene.

Crystalline derivatives of fullerenes. — Fullerenes are closed shell carbon molecules. The most abundant among them is C_{60}. The conjugated bond system makes C_{60} ideal precursors of ionic and covalent derivatives. In condensed state the rotation and the supramolecular interactions of the high-symmetry molecules enlarge the possibility of further structures. As a result, fullerenes have unusually large number of solid state derivatives, like alkali metal salts, polymers and cocrystals with a series of inorganic and organic molecules. There are materials with interesting properties in the group of A_xC_{60} compounds (A=Na, K, Rb, Cs). Several superconducting materials (A_3C_{60}), and also polymers with different dimensionality (RbC_{60}, Na_4C_{60}) were found. Most cocrystrals of fullerenes are host-guest or donor-acceptor materials. A couple of years ago we discovered a new family of cocrystals, the rotor-stator phases of fullerenes and cubanes. These materials consist of separated sublattices of rotating fullerene and static cubane components. In the prototype of this family C_{60} molecules form an expanded face centered cubic lattice in which cubane molecules occupy the octahedral voids. The topological recognition of the slightly concave faces of cubane (C_8H_8) and the convex surface of spherical C_{60} stabilizes the structure without preventing the rotation of fullerenes. Thus, the static cubanes behave like molecular bearings between the rotating fullerene molecules. A series of related cocrystals with higher fullerene and also with 1,4-disubstituted cubane components have similar structural characteristics but the influence of the lower symmetry gives rise to somewhat modified properties. A further point of interest of this family is the topochemical copolymerization of the cocrystals, induced by the decomposition of cubane at elevated temperatures. This year we have finished the structural studies on $C_{60}{\cdot}C_8H_8$ and, in the framework of an international collaboration, started the study on the dynamics of the related C_{70} derivative. We extended the family of the rotor-stator materials to new high-symmetry derivatives: the cubane and mesitylene cocrystals of the endohedral trimetallonitride compound of C_{80}. $Sc_3N@C_{80}{\cdot}C_8H_8$ has a rocksalt structure with static cubane and rotating fullerene molecules. At ambient temperature the Sc_3N unit also rotates inside the fullerene cage. We found that the Gd derivative has similar structure with interesting magnetic properties.

Carbon nanotubes and graphene. — We studied fullerenes and related compounds, carbon nanotubes and graphene, and hybrid materials containing other organic molecules beside them. We investigated systematically the fundamental properties of carbon nanotubes as function of diameter, chirality and doping; we detected a low-energy gap at terahertz frequency and nanotube vibrational modes in the infrared, supported by theoretical calculations. Many of our studies were devoted to following the dependence of spectroscopic features on temperature and pressure, thereby gathering information on the Jahn-Teller effect in fullerides as well as on the structure of encapsulated and double-walled nanotubes. Combining our methods with scanning probe spectroscopies, we could

[#] Ph.D. student

assign functionalized and doped areas on nanotubes. We also proposed a new application of functionalized nanotubes as "catchers" of metal ion pollutants in wastewater. Other supramolecular systems, hydrogen-bonded nucleic acid base-analogs, were studied by infrared spectroscopy and molecular dynamics calculations, to detect the "melting" temperature of hydrogen bonds.

Theory of structure solution at the atomic level. — *Charge flipping* is a simple, dual-space algorithm of structure determination that we have developed in the last few years. It is increasingly applied in a variety of cases, ranging from single crystals to powders, from periodic to aperiodic structures, from complete small-molecule arrangements to protein heavy-atom substructures – successful examples include some previously unsolvable zeolites and quasicrystals. In the past year we have developed a new variant of the charge flipping algorithm which efficiently handles the general problem of incomplete data. We have shown that in favourable cases a small-molecule structure can be solved by using only 1/8-th of the diffraction data compared to the requirement of current crystallographic practice. This result opens new routes for the application of the method.

Single molecule imaging. — The bottleneck of the structure solution of biological systems is the fact that not all specimens can be crystallized. Therefore, single molecules should be measured. However, small samples are severely damaged by the measuring process itself. Even the most often used x-rays destroy the sample during the collection of a diffraction pattern. However, with the introduction of x-ray free electron laser (XFEL) sources a new possibility appears: one might be able to do a measurement before the atoms have time to move. This means taking a diffraction pattern within a few femto-seconds. Since presently only a single source exists (LCLS), which produces proper pulses to do single molecule imaging, measurements are scarce. Modeling of data evaluation is very valuable. We studied classification, the first step of the data evaluation process. We worked out a new classification schema based on the rotational symmetry of the measurements and the spherical nature of the common part of 2D diffraction patterns. We demonstrated that it is possible to carry out the classification of 10^6 2D diffraction patterns modeled at realistic XFEL parameters.

Theory of phase transformations. — We have addressed competing fcc and bcc nucleation in alloys using a vector order parameter continuum model that relies on Ginzburg-Landau free energies of the liquid-fcc, liquid-bcc, and fcc-bcc subsystems, and determined the properties of crystal nuclei as a function of composition, temperature, and structure. With a realistic choice for the free energy of the fcc-bcc interface, the model predicts well the fcc-bcc phase selection boundary in the Fe-Ni system. We have used a simple dynamical density functional theory, termed the PFC method, for exploring the ubiquitous morphological changes in crystallizing systems with increasing thermodynamic driving force. This approach bridges the gap between molecular simulations and coarse-grained continuum models, while operating on diffusive time scales. A colloidal 'soft' material has been chosen as a model system for our investigation since there are careful colloidal crystallization observations at a particle scale resolution for comparison, which allows for a direct verification of our simulation predictions. We have particularly focused on a theoretically unanticipated, and generic, morphological transition leading to progressively irregular-shaped single crystals in both colloidal and polymeric materials with an increasing thermodynamic driving force. We have discovered a 'fast' mode of crystal growth at high driving force, suggested before in experimental colloidal crystallization studies, and found that the coupling of this crystal mode to the well-understood 'diffusive' or 'slow' crystal growth mode could greatly affect the crystal morphology at high thermodynamic driving force. In particular, understanding of this

interplay between the fast and slow crystal growth modes allows us to describe basic crystallization morphologies seen in both colloidal suspensions with increasing particle concentration and crystallizing polymer films with decreasing temperature: compact symmetric crystals, dendritic crystals, and fractal-like structures (Fig. 1). The same PFC approach has been used to investigate the structural aspects of crystal nucleation in undercooled liquids in 3D: It has been shown that the first appearing solid is amorphous, which promotes the nucleation of bcc crystals but suppresses the appearance of the fcc and hcp phases. These findings have been associated with features of the effective interaction potential deduced from the amorphous structure.

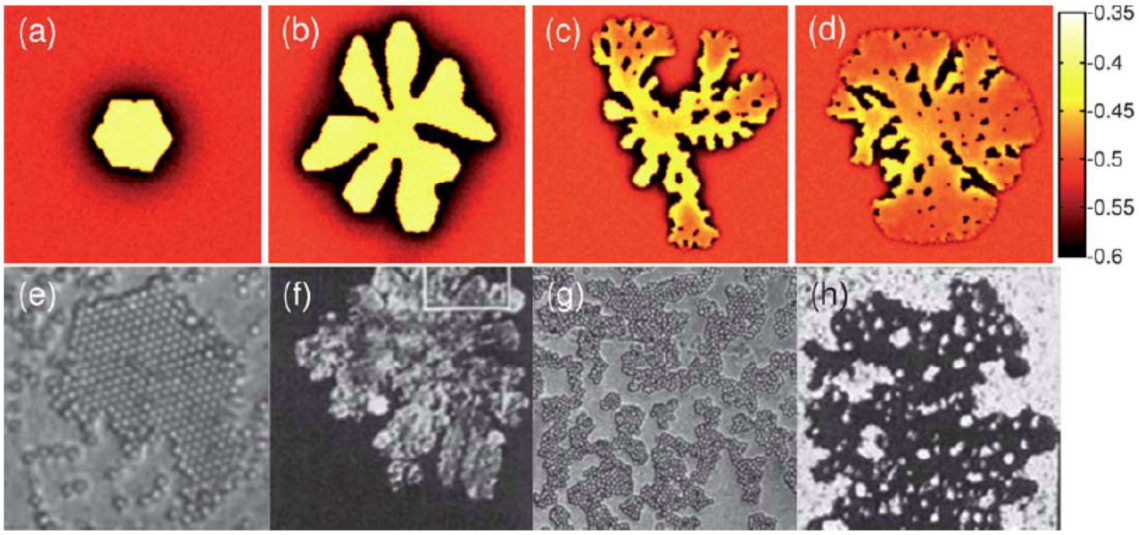

Fig. 1. *Solidification morphologies (a)-(d) as predicted by a simple dynamical density functional theory (E.2 and E.6) and (e)-(f) in colloid experiments (Skjektorp A T, Phys Rev Lett;* ***58****, 1444-1447, 1987).*

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Grants and international cooperations

OTKA K062588 Dynamics of complex systems (T. Pusztai, 2006-2011)
OTKA K72954 Rotor-stator phases of the fullerene-cubane system and related supramolecular materials (S. Pekker, 2008-2012)
OTKA K067980 New methods for solving the phase problem II. (G. Oszlányi, 2007-2012)
OTKA T075813 Polymerization in carbon nanostructures (K. Kamarás, 2009-2012)
OTKA K81348 Ultrafast diffraction imaging of single particles (M. Tegze, 2010-2014.)
ESA PECS Contract No. 4000104330/11/NL/KML: GRADECET-Phase-field modelling of columnar to equiaxed transition with fluid flow (L. Gránásy, 2011–2013).
CLS 14-3490 Investigation of the bonding structure of fullerene-cubane molecular crystals and its polymers (F. Borondics, Canada, 2011)
NFÜ TECH-09-A2-2009-0134, FIBERSC2 Development of fiber integrated nonlinear microendoscope based on new fiber laser technology, for pharmacological and diagnostic investigations (2009-2012, consortium leader: R. Szipőcs, Scientist-in-charge for RISSPO: K. Kamarás)
EU FP7-Marie Curie Initial Training Network PITN-GA-2008-215399: Cavity-confined luminophores for advanced photonic materials: a training action for young researchers (FINELUMEN) (Coordinator: N. Armaroli, CNR-ISOF, Bologna, Italy, representative of contractor: K. Kamarás)
Alexander-von-Humboldt Foundation Joint Research Project 3-Fokoop-DEU/1009755, 2006-2011: Electronic properties of doped C_{60} and nanotube compounds, principal investigators: K. Kamarás (Hungary), Rudolf Hackl (Walther-Meissner Institute, Bavarian Academy of Sciences, Garching, Germany)
FP7 PRE-XFEL 211604 Preparatory Phase of the European X-ray Free Electron Laser Facility (G. Faigel 2008-2011)
Participation in COMET K2 project A1.1.: Numerical Investigations on Dendritic Mushy Zones (T. Pusztai, 2009–2012)
Participation in EU FP7 NMP4-SL-2008/213669 ENSEMBLE Engineered Self-organised Multi-Component Structures with Novel Controllable Electromagnetic Functionalities (L. Gránásy, 2008–2012)

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Book chapter

E.26. Tóth GI, Pusztai T, Tegze G, Tóth* G, Gránásy L; Phase-field crystal modeling of homogeneous and heterogeneous crystal nucleation*;* In: *Containerless Undercooling of Drops and Droplets,* Ed: D. M. Herlach and D. M. Matson, Wiley-VCH GmbH & KGaA, Weinheim, ISBN 978-3-527-33122-2, accepted for publication

See also: T.15.

F. COMPLEX FLUIDS

Á. Buka, T. Börzsönyi, N. Éber, K. Fodor-Csorba, I. Jánossy, P. Salamon[#], B. Szabó[#], T. Tóth-Katona, A. Vajda

Synthesis. — A derivative of the methyl red azo-dye has been prepared for non-linear optical investigations. Different bent-core monomers and their mixtures have been prepared which were used in composite materials with magnetic nanoparticles. Reactive linear and bent core liquid crystals have also been synthesized for polymerization and preparation of liquid crystal elastomers.

Electric field driven pattern formation. — A detailed theoretical analysis of the flexoelectric instability of a planar nematic layer has been carried out in the presence of an alternating electric field of frequency f, which leads to stripe patterns (flexo-domains). This equilibrium transition is governed by the free energy of the nematic, which describes the elasticity with respect to the orientational degrees of freedom as well as the electric interactions. Surprisingly the limit $f \to 0$ is highly singular. In distinct contrast to the dc case, where the patterns are stationary and time independent, they appear at low f periodically in time as short flashes. Flexo-domains are in competition with the intensively studied electro-hydrodynamic instability in nematics, which represents a non-equilibrium dissipative transition. It has been demonstrated that f is a very convenient control parameter to tune between flexo-domains and convection patterns, which are clearly distinguished by the orientation of their stripes.

The temporal evolution of the spatially periodic electroconvection (EC) patterns has been studied within the period of the driving ac voltage by monitoring the light intensity diffracted from the pattern. Measurements have been carried out on a variety of nematic systems, including those with negative dielectric and positive conductivity anisotropy, exhibiting "standard EC" (s-EC), those with both anisotropies negative exhibiting "nonstandard EC" (ns-EC), as well as those with the two anisotropies positive. Theoretical predictions have been confirmed for stationary s-EC and ns-EC patterns. Transitions with Hopf bifurcation have also been studied. While traveling had no effect on the temporal evolution of dielectric s-EC, traveling conductive s-EC and ns-EC patterns exhibited a substantially altered temporal behaviour with a dependence on the Hopf frequency. It has also been shown that in nematics with both anisotropies positive, the pattern develops and decays within an interval much shorter than the period, even at relatively large driving frequencies.

Liquid crystal composite materials. — The influence of dodecanethiol functionalized gold nanoparticles (with diameter 3–5 nm) on the structural transitions has been investigated in a nematic liquid crystal 4-(trans-4'-n-hexylcyclohexyl)-isothiocyanatobenzene (6CHBT). It has been shown that the inclusion of gold nanoparticles increases the sensitivity of 6CHBT to the imposed external magnetic fields. Stable colloidal suspensions of neat and magnetite-labeled single-walled carbon nanotubes in 6CHBT have also been prepared. The morphology and the size distribution of the nanotubes have been determined by transmission electron microscopy. For the magnetite labeled nanotubes a significant increase of the saturation magnetization has been detected by a SQUID magnetometer. By measurements in electric and magnetic fields, the density of the anchoring energy at the nematic–magnetic particle boundary has been found higher for the liquid crystal doped with magnetite labeled nanotubes than that for suspension with

[#] Ph.D. student

neat nanotubes. The nematic to isotropic phase transition temperature of 6CHBT doped with magnetic nanoparticles of different shape has been monitored by precise capacitance measurements in external magnetic fields up to 12 T. A magnetic-field induced shift in the transition temperature has been first observed in a calamitic liquid crystal doped with rod-like magnetic particles.

Interactions at liquid crystal surfaces. — Optically induced instabilities were observed in nematic liquid crystals sandwiched between a photosensitive layer and a reference plate. The instabilities occurred when the light entered the cell from the reference plate and its polarization was parallel to the director alignment at the entrance face. Two kinds of patterns were detected: a static and a dynamic one (Fig.1). The underlying mechanism of these pattern formations is the coupling between the director orientation on the photosensitive plate and the polarization direction of the light on the same plate.

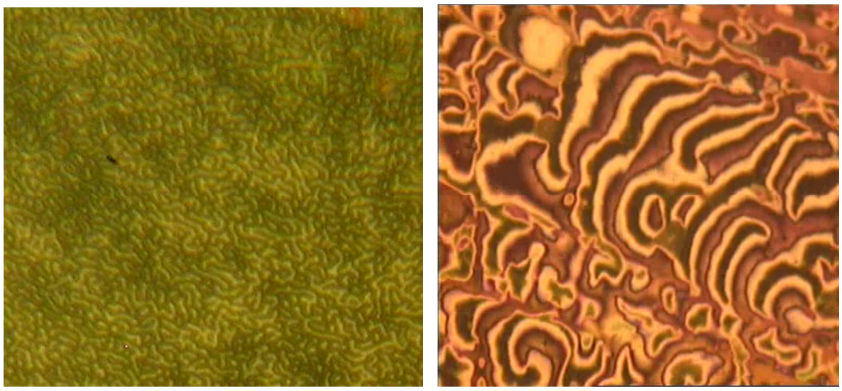

Fig. 1. *Optically induced static (left panel) and dynamic (right panel) patterns.*

Granular dynamics. — A block of granular material consisting of two horizontal layers with different friction was deformed by moving the bottom wall of the container (see Fig. 2). The deformation zone finds an optimal path in the material by escaping the lower (high friction) layer and staying in the low friction layer near the layer boundary (Fig. 2.c). The formalism describing the selection of the optimal path is very similar to that of light propagation through inhomogeneous media.

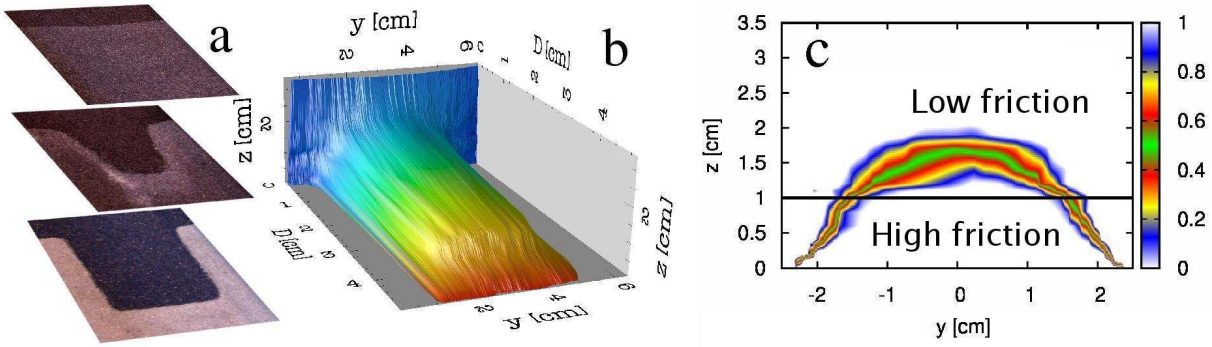

Fig. 2. *A layered granular material is deformed by moving the bottom wall of the container. (a-b) The displacement is visualized by using colour samples and excavating the material layer by layer. The deformation zone (see panel c) does not remain at the bottom of the cell (this would be the shortest way connecting its two ends) but escapes the high friction layer and stays in the low friction layer near the layer boundary (horizontal black line).*

Resonant silo discharge - called silo music - has been investigated experimentally. Grain motion has been detected with high speed imaging, while the systems resonance was monitored with a microphone and piezoelectric accelerometers. It was found that the grains do not oscillate in phase at neighbouring vertical locations; rather information

propagates upward in this system in the form of sound waves. It was shown that the wave velocity is not constant throughout the silo; it considerably increases toward the lower end of the system, suggesting increased pressure in this region, where the flow changes from cylindrical to converging flow. Grain oscillations exhibit a stick-slip character only in the upper part of the silo.

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Grants and international cooperations

OTKA K 81250 Electro and photomechanical effects in organic soft materials (I. Jánossy, 2010-2014)

COST D35 WG 13-05 Molecular switches based on liquid crystalline materials (K. Fodor-Csorba, 2005-2011)

NKTH TÉT AR-3/2008 (Hungarian-Argentinian bilateral) Transient and metastable states (Á. Buka, 2009-2012)

HAS-ASCR (Hungarian-Czech bilateral) Synthesis and characterization of reactive mesogenic monomers, and their utilization in crosslinked systems (T. Tóth-Katona, 2010-2012)

HAS-INSA (Hungarian-Indian bilateral) Experimental and theoretical studies on soft condensed matter (N. Éber, 2010-2012)

HAS-SASA (Hungarian-Serbian bilateral) Structural studies of liquid crystalline mixtures (N. Éber, 2010-2012)

HAS-SAS (Hungarian-Slovak bilateral) Anisotropic magnetic fluids (N. Éber, 2010-2012)

Long term visitors

— Laura Olivia Palomares: Instituto de Física, Universidad Nacional Autónoma de México, Mexico D.F., Mexico, January 02 – December 31, 2011 (host: Jánossy I)

— Prof. Antal Jákli: Liquid Crystal Institute, Kent State University, Kent, USA, June 20 – July 23, 2011 (host: Éber N)

— Jakub Kolacz: Kent State University, Kent, USA, June 01 – July 15, 2011 (host: Éber N)

— Prof. David Statman: Allegheny College, Meadville, USA, July 04 – August 15, 2010 (host: Jánossy I)

— Kaitlin Wozniak: Allegheny College, Meadville, USA, July 04 – August 20, 2011 (host: Jánossy I)

— Andrew Jockers: Allegheny College, Meadville, USA, July 04 – August 20, 2011 (host: Börzsönyi T)

— Robert Pettit: Allegheny College, Meadville, USA, July 04 – August 20, 2011 (host: Éber N)

— Sarah Bottini: Allegheny College, Meadville, USA, July 04 – August 20, 2010 (host: Éber N)

Publications

Articles

F.1. Kopčansky* P, Tomašovičová* N, Koneracká* M, Timko* M, Mitróová* Z, Závišová* V, Éber N, Fodor-Csorba K, Tóth-Katona T, Vajda A, Jadzyn* J, Beaugnon* E, Chaud* X; Structural phase transition in liquid crystal doped with gold nanoparticles; *Acta Phys Pol A*; **118**, 988-989, 2010

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F.4. Krekhov *A, Pesch* W, Buka A; Flexoelectricity and pattern formation in nematic liguid crystals; *Phys Rev E;* **83,** 051706/1-13, 2011

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F.8. Jánossy I, Fodor-Csorba K, Vajda A, Palomares* LO; Light-induced spontaneous pattern formation in nematic liquid crystal cells; *Appl Phys Lett;* **99**, 111103/1-3, 2011

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F.11. Obadović* DŽ, Stojanović* M, Jovanović-Šanta* S, Cvetinov* M, Lazar* D, Vajda A, Éber N, Ristić* I; Study of binary cholesteric liquid crystalline mixtures doped with some chiral nonmesogenic estradiol derivatives; *Mol Cryst Liq Cryst;* **547**, 46-53, 2011

F.12. Obadović* DŽ, Stojanović* M, Cvetinov* M, Vajda A, Éber N, Lazar* D; The study of phase transition in some irradiated cholesteric liquid crystalline mixtures; *Russ J Phys Chem A*; **85**, 110-113, 2011

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F.13. Bata L; "Ne erőltessenek rám semmit" ("Don't enforce anything on me", in Hungarian); *Természet Világa*; **142**, Special issue, pp. 72-75, 2011

G. RADIOFREQUENCY SPECTROSCOPY

G. Kriza, P. Bánki, M. Bokor, P. Matus, B. Sas, K. Tompa, T. Verebélyi[#], *F.I.B. Williams*

Hydration of proteins associated with Parkinson's disease. — Parkinson's disease (PD), like Alzheimer's disease (AD), is a lingering neurodegenerative disease that induces degeneration of substantia nigra in the brain in people typically older than age 60. The loss of dopaminergic neurons causes movement disorders. PD is characterized by the presence of cytoplasmic neuronal deposits, so-called Lewy bodies (LBs). The major component of LBs is α-synuclein, which forms ordered amyloid fibrils; in fact, α-synuclein immunoreactivity in LBs is the pathological hallmark of PD. Besides the wild-type variant, α-synuclein also has several inherited, familial mutations associated with PD, such as A53T, A30P, and E46K. Therefore, unraveling the structural effects of these mutations has basic implications in understanding the molecular foundations of the disease.

α-synuclein is a small, highly soluble, heat-stable protein expressed at high levels in the brain, where its normal function is not fully understood. The wild-type protein and its mutants show different characteristics in many aspects, such as the rate of fibril formation and morphology, which underscores that these mutants are important in the development of PD. In vitro, A53T forms fibrils the fastest and wild-type is the slowest of all. The reasons for these observed differences are not clear, but they are probably related to the effect of mutations on both the solution structure of the protein and the interresidue interactions critical for amyloid formation.

We addressed this issue through comparing details of the hydration of wild-type α-synuclein and its A53T mutant by a combination of wide-line NMR, differential scanning calorimetry (DSC), and molecular dynamics (MD) simulations. All three approaches suggest a hydrate shell compatible with a largely disordered state of both proteins. Its fine details, however, are different, with the mutant displaying a somewhat higher level of hydration (Fig.1), suggesting a bias to more open structures, favorable for protein-protein interactions leading to amyloid formation. These differences disappear in the amyloid state (Fig.2), suggesting basically the same surface topology, irrespective of the initial monomeric state. Our experiments suggest that familial mutations cause small but significant local and global perturbations in the structural ensemble of α-synuclein, which are probably relevant with respect to their enhanced amyloidogenic potential. Our study adds a new dimension to the structural interpretation of amyloid formation by close inspection of the hydration properties of wild-type α-synuclein and the A53T mutant with the help of a combination of wide-line NMR and DSC.

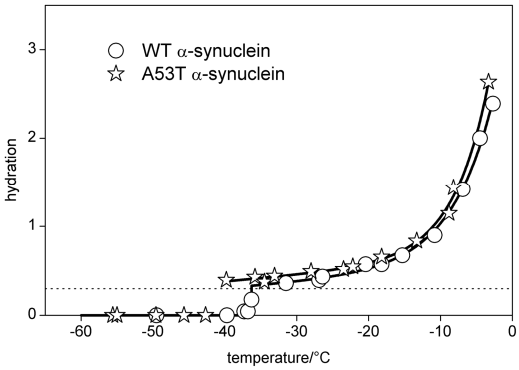

Fig. 1. *Temperature dependence of hydration as measured by ^1H NMR for 25 mg·cm^{-3} α-synuclein dissolved in pure water of the wild and A53T variants. The dotted line is at the hydration level of 0.3 g water/g protein; solid lines are guides to the eye.*

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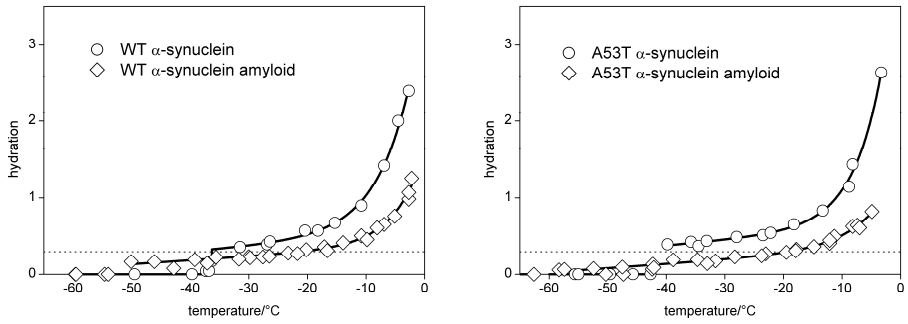

Fig. 2. *Comparison of the temperature dependence of hydration as measured by ^1H NMR for wild–type (left) and A53T (right) α-synuclein and its amyloid dissolved in pure water. The protein concentration is 25 mg·cm^{-3} in each case. The dotted line is at the hydration level of 0.3 g water/g protein; solid lines serve as guides to the eye.*

Data processing and evaluating software. — A computer program has been developed for instant processing and evaluation of the measured raw NMR data. The program can also be used for the analysis of the measured NMR parameters and the statistical characterization of the spectra.

NMR probe for measurements at liquid He temperature. — An NMR-probe has been designed and built which can be used between 300 K and temperatures as low as 4 K.

Elementary excitations in graphene. — Graphene has opened new avenues in many scientific disciplines and in particular holds promise of important applications such as terahertz electronics. From the point of view of fundamental solid state physics, its most exciting property is its quasiparticle spectrum analogous to that of massless Dirac fermions which is the consequence of the Fermi energy lying at the points where the energy bands cross and the dispersion is linear: any excess electron or hole propagates at fixed speed independent of energy as for free particles in the extreme relativistic regime (e.g. neutrinos). This relativistic dynamics alters the properties of the plasmon and especially the magneto-plasmon collective charge oscillations which we are engaged in investigating by near field THz spectroscopy.

In conjunction with the Nanoelectronics Group of the Service de Physique de l'Etat Condensé (SPEC) at CEA-Saclay, we have set up a swept frequency experiment over 2-50 GHz at 4 K in high magnetic fields at Saclay to investigate the dynamics of charge carriers in the quantum Hall regime where resonances from one dimensional chiral edge magnetoplasmon excitations are expected to arise. The 40 micron exfoliated graphene sample is placed in a break made in a micro fabricated coplanar waveguide whose transmitted power is measured. The sample response is identified by modulating the graphene electron density distribution with a side gate and detecting the transmitted power at the modulation frequency. Preliminary results on the fixed frequency graphene response as a function of magnetic field reveal two different components. One, dominant under large side gate voltage, is symmetric in B and the other, visible only at low gate voltage modulation, shows reproducible fluctuations which are not symmetric in B to $-B$, but which do obey the reciprocity relation on simultaneous inversion of source and detector and of sign of B. The first part is thought to be related to the bulk conductivity and the second to chiral carrier dynamics close to the edge, the fluctuations of impedance originating in the scattering from localized states.

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Joint Project supported by the Korean Research Council of Fundamental Science & Technology (KRCF) and HAS (Hungarian project leader: P. Tompa, Institute of Enzymology, BRC, HAS; participating RISSPO scientists: K. Tompa, M. Bokor, P. Matus, T. Verebélyi, 2011-2012)

Publications

Articles

G.1. Házy* E, Bokor M, Kalmár* L, Gelencsér* A, Kamasa P, Han* KH, Tompa K, Tompa* P; Distinct hydration properties of wild-type and familial point mutant A53T of α-synuclein associated with Parkinson's disease; *Biophysical Journal;* **101**, 2260-2266, 2011

Book chapters

G.2. Nagy* K, Horváth* Z, Tompa K; Fizika (Physics, in Hungarian); In: *Akadémia, a nemzet tanácsadója. Tanulmánykötet Glatz Ferenc 70. születésnapjára* (The Academy, the nation's advisor. Essays on the occasion of the 70th birthday of F. Glatz, in Hungarian); Editor in chief: I. Láng (MTA Társadalomkutató Központ, Budapest); pp. 681-693, 2011

G.3. Tompa K, Bokor M, Tompa* P; Wide-line NMR and protein hydration; In: *Experimental tools for the intrinsically disordered protein analysis, Chapter 13;* Eds: V.N. Uversky, A.K. Dunker (Springer Science+Business Media, LLC, New York, NY, USA), Vol. 1 (accepted for publication)

Other

G.4. Az „ötös faktor" – Beszélgetés Tompa Kálmánnal (The factor five – Discussion with K. Tompa, in Hungarian, interview by Á. Simon); *Természet Világa, Természettudományi Közlöny* **142**, Special issue I, pp. 76-79, 2011

H. ELECTRODEPOSITED NANOSTRUCTURES

L. Péter, I. Bakonyi, J. Dégi[#], K. Neuróhr[#], L. Pogány, B. Tóth[#]

Depth profile analysis of electrodeposited multilayers. — The co-operation with the Nuclear Research Institute of the HAS (Debrecen, Hungary) was successfully continued for the reverse depth profile analysis of various electrodeposited alloys. Several alloy systems were studied in which the minor alloy component could be deposited preferentially with respect to the main component (Ni). In all cases, the preferentially deposited alloying element was accumulated in the near-substrate zone, which ranged to about 150 nm in each case. When the minor component was either Cu or Cd, it was observed that the partial current density of the preferentially deposited components was smaller in the steady-state deposition regime than in the absence of the main component. When Ni was alloyed with a minor amount of Sn, the deposit structure proved to be very sensitive to the concentration of the alloying element. At small Sn^{2+} concentration (c = 3 mM), the composition depth profile showed a small Sn accumulation in the near-substrate zone, while the steady-state zone exhibited a low Sn molar fraction of about 1 at%. When the Sn^{2+} concentration in the electrolytic bath was increased to 10 mM, the composition ratio of the elements in the deposit was inverted, and Sn-rich deposit was obtained, in spite of the large Ni^{2+} concentration of the bath. In parallel to the increase of the Sn molar fraction in the deposit, it was observed that the Cu content of the substrate migrated to the deposit. A particularly interesting composition depth profile was found when both Cu and Co were alloying components in Ni-rich alloys. When the deposit was prepared with the help of a Si/Cr/Ag substrate, the composition analysis of the initial zone revealed that the accumulation of the alloying elements took place in the order of their deposition preference. The same type of spontaneous modulation was observed earlier for the Fe-Co-Ni alloys, too.

Electrodeposition of Co-Ru alloys. — The electrochemical codeposition of Co and Ru was systematically studied with solutions of wide composition ratio of Co^{2+} and Ru^{3+}. The codeposition of Co besides Ru was found to be anomalous because Co was codeposited at potentials where the deposition of pure Co is not possible. However, the deposition of pure Ru could not be achieved with a significant current efficiency. As the deposition temperature was increased to 50 ^{o}C, the deposition rate of both Co and Ru increased. The morphology of the deposits was determined mainly by the deposit composition and the deposition temperature was of minor importance only. At low Co content (i.e., at low deposition current density), the coating was discontinuous, and round-shaped voids could be observed which corresponded to the impact of the hydrogen bubbles. As the Co content of the deposit increased, the continuity of the deposits improved significantly. At Co contents above 60 at.%, the deposits were uniform but they exhibited fracture lines due to the residual stress. The crystalline structure of the deposits corresponded to a single hexagonal close-packed phase with varying lattice parameter as a function of the deposit composition.

Magnetoresistance and surface roughness of ultrathin electrodeposited Co/Cu multilayers. — Co/Cu multilayer samples were prepared by electrochemical deposition onto Si/Cr/Cu substrates. The properties of the deposits were very sensitive to the number of layers, to the layer sequence and the nature of the terminal layer. A single Cu-capped Co layer could also lead to giant magnetoresistance (GMR); nevertheless this behaviour is

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expected to multilayer systems only. The occurrence of the GMR in this case could be explained with the fact that the hindered nucleation of the Co layer leads to separated Co islands in the early phase of the deposition. With the increase of the bilayer number, the GMR increases, indicating the suppression of the shunt effect of the substrate. The maximum GMR value corrected for the shunt effect of the substrate was achieved at about 50 nm total multilayer thickness. At higher total thicknesses, the ratio of the superparamagnetic contribution to the GMR increased nearly linearly, while the ferromagnetic contribution slowly declined. The surface roughness study of the same multilayers showed that a saturation roughness value is achieved for a much lower thickness, and it did not change with increasing total multilayer thickness. This indicates that the surface roughness alone cannot be responsible for the changes observed in the GMR. The surface roughness of the Cu-terminated multilayer deposits always exceeded the roughness of the Co-terminated ones (at the same total thickness). This could be partly explained with the Co to Cu exchange at the deposit surface between the end of the deposition and the removal of the sample from the electrolyte solution. The impact of the exchange reaction on the GMR was also studied systematically. The exchange reaction was found to be deleterious for the GMR.

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Grants and international cooperations

OTKA K 75008 Giant magnetoresistance (GMR) in electrodeposited multilayers (I. Bakonyi, 2009-2011)

OTKA NN 79846 Correlation of microstructure and magnetoresistance in nanoscale multilayers (L. Péter, 2010-2011; collaborating partner: Technical University Freiberg, Germany)

OTKA NN 79943 Formation mechanism, microstructure evolution and reactivity of simplectites created during garnet breakdown processes (Principal investigator: K. Török, Eötvös Loránd Geophysical Institute of Hungary; SZFKI participant: J. Dégi, 2010–2014)

DUNAFERR contract Design and construction of a laboratory-scale workstation simulating the industrial pickling of steel (L. Péter, 2010-2011)

Publications

Articles

H.1. Neuróhr K, Csik* A, Vad* K, Bartók A, Molnár* G, Péter L; Composition depth profile analysis of electrodeposited alloys and metal multilayers: the reverse approach; *J. Solid State Electrochem.;* **15**, 2523-2544, 2011; DOI 10.1007/s10008-011-1465-x

H.2. Péter L; Comment on "Magnetoresistance of CoNiCu/Cu Multilayers Electrodeposited from Electrolytes with Different Ni ion concentrations; (J.

Electrochem. Soc. **157**(10) D538-D545 (2010).); *J Electrochem Soc;* **158**, S1-S2, 2011

H.3. Rafaja* D, Schimpf* C, Schucknecht* T, Klemm* V, Péter L, Bakonyi I; Microstructure formation in electrodeposited Co-Cu/Cu multilayers with GMR effect: influence of current density during the magnetic layer deposition; *Acta Mater.*; **59**, 2992-3001, 2011

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H.7. Esmaili* S, Bahrololoom* ME, Péter L; Magnetoresistance of electrodeposited NiFeCu alloys. *Thin Solid Films*, accepted for publication; DOI: 10.1016/j.tsf.2011.11.022

See also: D.1., I.6.

I. METALLURGY AND MAGNETISM

L.K. Varga, É. Fazakas[#], G. Gulyás[#], P. Kamasa, G. Konczos, Gy. Kovács[+]

Metallurgy. — Looking for light alloys with high strength at high temperatures, Al-Ti based alloys were prepared by ball milling and subsequent consolidation of the powders. The following compositions were successfully prepared in amorphous state: $Al_{50}Ti_{50-X}Ni_X$ (x=0, 5, and 10), $Al_{55}Ti_{30}Cr_{15}$ and $Al_{45}Ti_{40}Cr_{15}$. The alloy ingots were prepared by induction melting in water-cooled copper mould and the ball milling was accomplished in two high-energy milling devices: a SPEX-8000 shaker mill and a Fritsch planetary ball mill. Since the Al-Ti based amorphous alloys could not be prepared by the usual melt-spinning method, bulk amorphous and partially nanocrystalline tablets were prepared by hot pressure consolidation and characterized by usual metallographic methods.

A series of β-SiC nanopowders was produced by two different experimental techniques: 1) reactive bonding by inductive heating and subsequent wet chemical etching, and 2) by mechanical alloying in SPEX-8000 shaker. The latter technique is suitable to be scaled up for practical applications. Both samples were characterized and evaluated by Research Topic T, as part of the Momentum programme.

Soft magnetic nanocrystalline alloys. — Substitution of some of the Fe with Co in partially devitrified Si-free Nanoperm-type alloys improves their soft magnetic properties, increases the Curie temperature of the amorphous matrix, and allows casting in air. A new, Si-free nanocrystalline alloy with the composition $(Fe_{100-x}Co_x)_{84.5}Nb_5B_{8.5}P_2$ (x = 20, 40, 60) was prepared and investigated The novel composition was published under the name Pyroperm, emphasizing the higher working temperature limit as compared to the existing similar alloys.

Seeking for high saturation magnetization nanocrystalline alloys, a series of Nb-free alloys like $Fe_{83.7}B_{14.8}Cu_{1.5}$, $Fe_{82.7}Si_2B_{14}Cu_{1.3}$ and $Fe_{80.6}Si_5B_{13}Cu_{1.4}$ was investigated. Saturation induction as high as B_{2000} = 1.9 T could be obtained at H_c = 15 A/m for optimal annealing conditions (390 ^oC /30 min). Continuing former work on mixed B- and P-based alloys, following Makino's personal communication novel high saturation magnetization nanocrystalline alloy compositions ($Fe_{85}Si_2B_8P_4Cu_1$) were prepared and their optimal heat treatment characteristics were established. Magnetic paramaters such as B_{800} = 1.85 T, H_c = 3 A/m and $W_{1.7/50}$ = 0.4 W/kg could be obtained experimentally, resulting the best figures for the time being in case of soft magnetic materials for network-frequency applications.

For high-frequency applications, a new core construction was designed which consisted of stacked toroidal sheets instead of the usual wound ribbon structure. In addition, a large DC biasing field was applied perpendicular to the sheet surface, tilting the almost saturated magnetization out of plane. The exciting AC field was applied along the toroid, i.e., in longitudinal direction which produces a longitudinal magnetization by rotation of the out-of-plane magnetization (Fig. 1). The dominating rotational magnetization process results in reduced coercivity and flattened magnetization curve (Fig. 2). The relative permeability could be diminished by more than two orders of magnitude (from 60 000 to 700). Correspondingly, the eddy current frequency limit (where the imaginary part of the permeability is maximum) was shifted from 60 kHz to 1 MHz.

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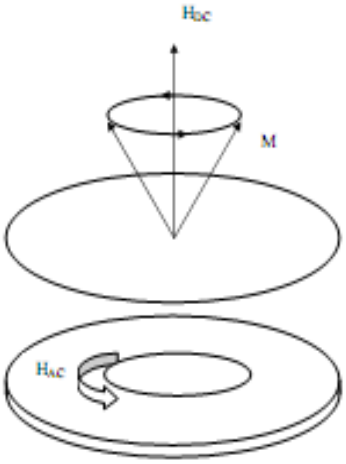

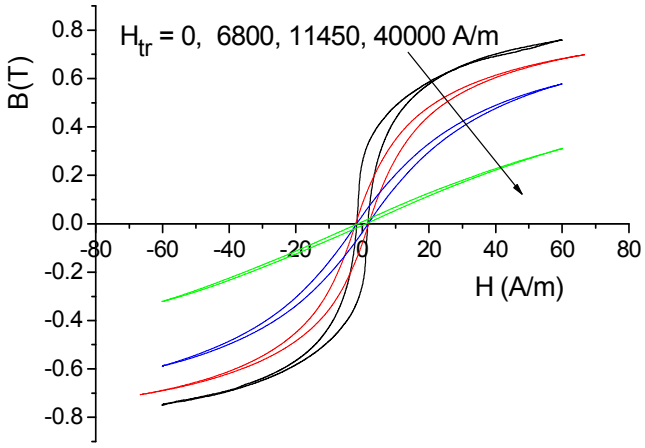

Fig.1. *The core was prepared by stacking up toroidal sheets (D_{ext} = 17.5 mm, D_{int} = 8.5 mm) cut from a 20 mm wide Finemet ribbon of 22 μm thickness. Resulted height of the toroid was 5 mm.*

Fig.2. *Flattening of the hysteresis loop due to the transversal DC field applied perpendicular to the sheet of the toroid. Only some selected loops are shown.*

Low-temperature calorimetric method: DSC characterization of protein aqueous solutions. — Calorimetric method and instrumentation were worked out and applied for the investigation of aqueous solutions of proteins. Thermal effects were analyzed by heat-flux-type DSC cell designed for temperature range from the boiling point of water down to 120 K. The achieved sensitivity of heat flow rate (*HF*) of the instrument is better than 50mW tested using 1 ml of 150 mM aqueous solution of NaCl. From the integral value of *HF,* the total enthalpy change ΔH_{total} and the enthalpies of transitions were separated from the heat capacities. Using the method, several types of proteins (BSA, ERD10, UBQ, α-, β-casein, and WT, A53T, A30P, E46K α-synuclein mutants) were investigated in that temperature range. Results obtained for α- and β-casein are shown in detail in Fig. 3 as an illustrative example.

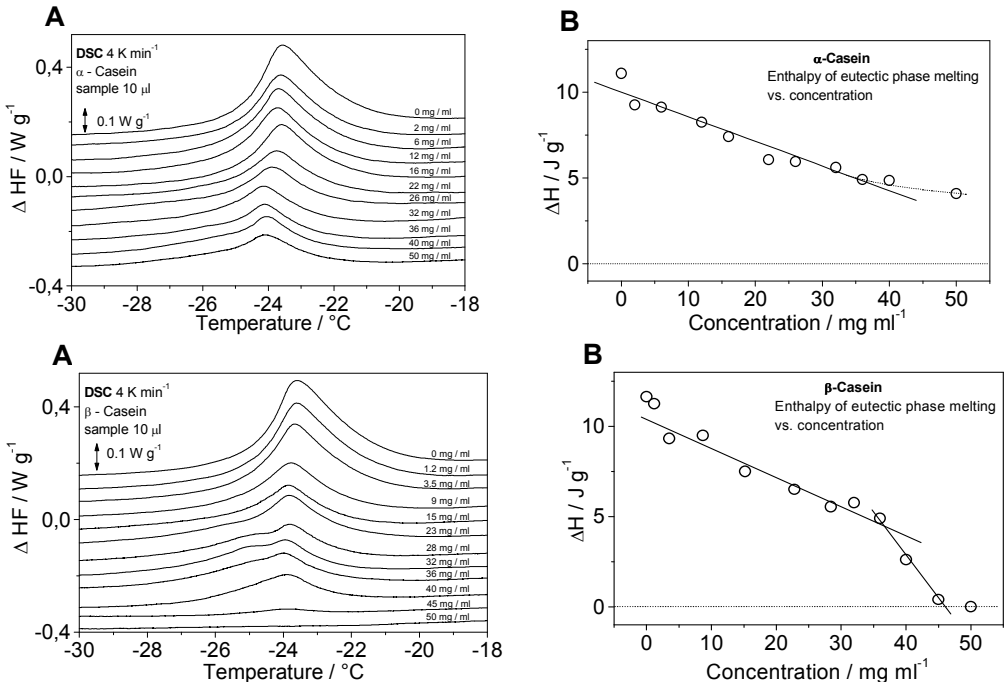

Fig. 3. *Thermographs showing a small endothermic peak (SEP) obtained during melting of eutectic phase of α- and β-casein dissolved in Tris-buffer for several concentrations ranging from 0 to 50 mg/ml (panel A). Enthalpy of SEP vs. concentration (panel B).*

Potential applications include (*i*) the distinction between the solvent-accessible surfaces of globular and intrinsically disordered proteins, (*ii*) the distinction between protein mutants, and (*iii*) the identification of monomer and polymer protein states. This method provides the possibility of studying the polymerization process (amyloid formation) and the *in-situ* investigation of its reason and circumstances.

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Grants and international cooperations

OTKA K73451 Preparation and investigation of Al- and Ti-based bulk amorphous and nanostructured composites (L.K. Varga, 2008-2011)

HAS-BAS Hungarian-Bulgarian Academy Exchange Programme: Glass-forming ability, structural relaxation and (nano)crystallization of ribbon-like and bulk amorphous and nanocrystalline alloys on the basis of Fe, Co, Ni, Zr and Al metals for mechanical and magnetic applications, studied by thermoanalytical, structural and magnetic measurements (L.K. Varga, 2009-2011)

HAS-SAS Hungarian-Slovakian Academy Exchange Programme: Study of physical properties of special magnetic materials (L.K. Varga, 2010-2012)

HAS-PAS Hungarian-Polish Academy Exchange Programme: Investigation of thermo-physical properties of coatings (P. Kamasa, 2008-2013)

HAS-RAS Hungarian-Russian Academy Exchange Programme: Calorimetric study of phase transformations (P. Kamasa, 2008-2013)

HAS-RAS Hungarian-Romanian Academy Exchange Programme: Structure, thermal and mechanical properies of amorphous and nanocrystalline Al-base alloys obtined by arc melting and mechanical alloying (É. Fazakas, 2008-2011)

TOMMY-INVEST ELECTRONICS LTD. Testing, designing and producing inductive cores for the inductive electronic component market (Project leader: L.K. Varga, 2011)

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I.8. Srivastava* SK, Srivastava* VK, Varga LK, Khovaylo* VV, Kainuma* R, Nagasako* M, Chatterjee* R; Systematic study of structural, transport, and magnetic properties of $Ni_{52+x}Mn_{26-x}Al_{22}$ ($1 \leq x \leq 5$) melt-spun ribbons; *J Appl Phys;* **109**, 083915/1-8, 2011

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I.10. Kane* SN, Tripathi* S, Coisson* M, Olivetti* ES, Tiberto* P, Vinai* F, Baricco* M, Fiore* G, Apolinário* A, Sousa* CT, Araujo* JP, Varga LK; Microstructure and magnetic properties of $(Fe_{100-x}Co_x)_{84.5}Nb_5B_{8.5}P_2$ alloys; *J All Comp;* accepted for publication

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See also: D.1., G.1., T.15.

J. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

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The 10 MW Budapest Research Rector (BRR) with its experimental facilities is a unique large-scale facility in the Central European region, a basis for domestic and international user community to serve for exploratory and applied research as well as for methodical developments. We operate a number of neutron scattering instruments (small angle scattering spectrometer, diffractometers, reflectometers, three-axis spectrometers). These devices have been used during this year to perform an important number of experiments. Here we present results of a study on a class of steels important for engineering sciences and an other breakthrough experiment in high resolution diffraction technique.

Residual stress measurements in metal standards. — The deep penetration of thermal neutrons into the bulk of material makes neutron diffraction a powerful tool for the residual stress measurement by the high precision determination of lattice parameters. Such non-destructive validation plays an important role in engineering sciences. For a series of "standard metal" samples a worldwide Round Robin test was performed; here we used the cold neutron triple axis spectrometer ATHOS in order to validate the procedure followed with our instrumental setup. ATHOS is an instrument with high flexibility and a relatively big sample table for investigation industrial samples. A vertically focusing PG (pyrographite) monochromator provides continuously changeable wavelength. The detector is a 200x200 mm position sensitive delay line type detector. The Round Robin sample was VAMAS Aluminium Ring & Plug Aluminium Ring & Plug Set.

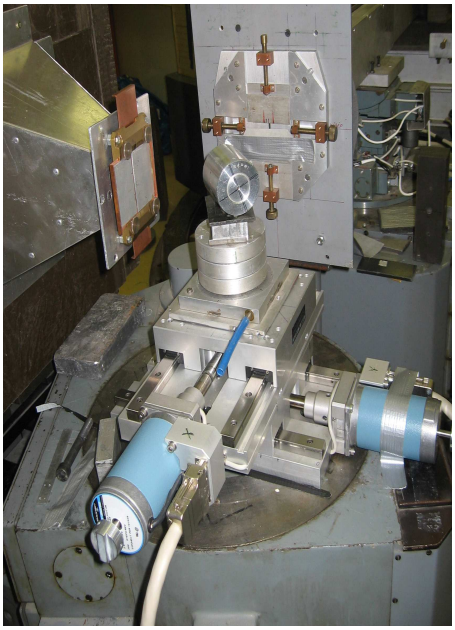

Fig. 1/a

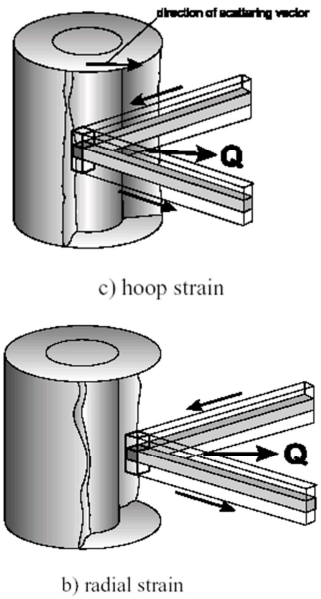

Fig. 1/b

Fig. 1/a *shows the experimental setup, and the scheme for measuring radial and hoop stresses are shown in* ***Fig. 1/ b****. For stress measurement we used 111 reflection using a gauge volume determined by the incident beam 20x3mm (HxW) and by the outgoing beam 20x3mm (HxW) at the detector direction. At 111 reflection*

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we used the wavelength of 0.33 nm giving us the 90 deg scattering angle.

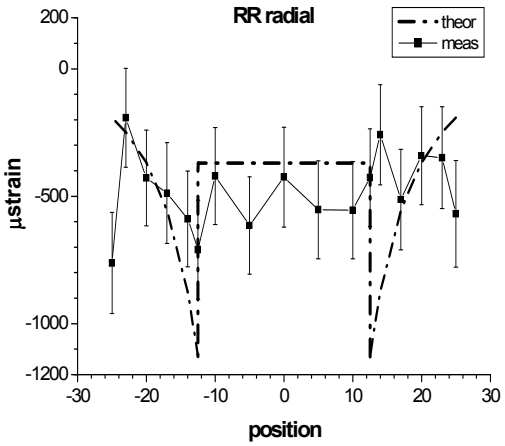

Fig. 2a. *Measured and calculated radial strain.*

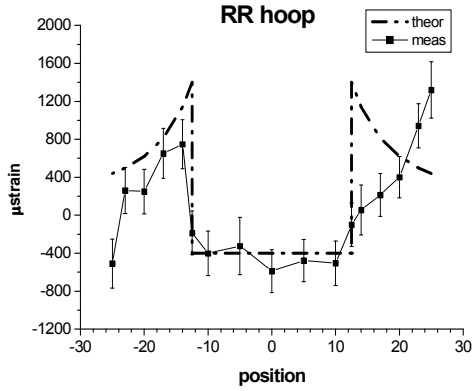

Fig. 2b. *Measured and calculated hoop strain.*

The measured strain data fit well to the results measured elsewhere of the Round Robin series. It is seen that the strain fits well on the negative side of sample position, while on the positive side the fit is rather poor due to longer beam path in the sample well corresponding to the peak intensity weakening. In our case the used wavelength 0.33 nm results higher absorption then the usually applied thermal beam (0.1-0.2 nm), the used geometry, however is more comfortable. We have made another improvement, too: using the 004 reflection of the PG monochromator results in a much less error bar with no substantial intensity loss.

Time-of-Flight (TOF) method. — For neutron diffraction this is a very efficient alternative to the crystal monochromator technique. High performance in diffraction is the most basic goal and a requirement for all neutron sources now or in the future. A technique to achieve it is of central importance for the new generation of continuous or long pulse sources. In collaboration with Helmholz Zentrum Berlin (HZB) (then Hahn-Meitner-Instituts Berlin, HMI) the Budapest Neutron Center (BNC) undertook to develop powerful TOF diffraction for both its own use and with the perspective of establishing a continuous source for the foundations of TOF diffraction. Based on this, last year a BNC-HZB team at Budapest successfully implemented and tested experimentally the special chopper system capable of turning a long pulse spallation source into an ideal short pulse source with flexible tunable pulse length for neutron diffraction work. This Wavelength Frame Multiplication (WMF) method allowed producing pulsed white neutron beams of any desired wavelength band effectively, by seamlessly stitching together a series of narrower wavelength bands from a series of pulses emanating from a pulse shaping chopper. This year the experiments using the TOF Diffractometer at BNC in unconventional modes of operation emulating long pulse sources successfully provided the proof of WMF method. It was shown that the combination of the neutron spectra coming from different chopper pulses into a single, broadest band diffraction pattern can be achieved with such perfection that the results of this combination display no difference at all compared to a diffraction pattern that would come from a single pulse. The WMF method is actually a variant of the by now fully developed Repetition Rate Multiplication multiplexing technique for neutron spectroscopy at pulsed sources. It has became the state-of-the art standard for TOF spectrometers such as LET at ISIS (Rutherford Appleton Laboratory in Oxfordshire, UK),

AMATERAS and 4 Seasons at J-PARC (Tokai, Japan) after it had been first demonstrated fully at the BNC TOF facility.

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Grants and international cooperations

EU-FP7-CP-CSA-INFRA-2008-1.1.1 Number 226507-NMI3 – Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy (J. Füzi, 2009-2012)

EU-FP7 – CHARISMA – Cultural Heritage Advanced Research Infrastructures: Synergy for a multidisciplinary approach to conservation/restoration (L. Rosta, 2009-2013)

OM-00079/2008/KPI (Jedlik) Research and Development of Marketable Materials and Technologies for Neutron Instrumentation (L. Rosta, 2008-2011)

NAP VENEUS05 OMFB-06482/2008 Visegrád Cooperation for Development and Application of Neutron Spectroscopy Techniques in Multidisciplinary Research (L. Rosta, 2008-2011)

OTKA-A08-3 OMFB-00590/2010 Structures and dynamics of self-organized lamellar molecular systems (F. Mezei, 2010-2012)

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Articles

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J.7. Gallová* J, Uhríková* D, Kučerka* N, Svorková* M, Funari* SS, Murugova* TN, Almásy L, Mazúr* M, Balgavý* P; Influence of cholesterol and beta-sitosterol on the structure of EYPC bilayers; *J Membrne Biol*; **43**, 1-13, 2011

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K. NEUTRON SCATTERING

L. Pusztai, M. Fábián[+], I. Harsányi, P. Jóvári, L. Kőszegi, Gy. Mészáros, V. Mile[#], Sz. Pothoczki, E. Sváb, L. Temleitner

Liquids. — We have performed a series of computer simulations on the three lowest *aliphatic alcohols*, *methanol, ethanol* and *1-propanol*, applying Reverse Monte Carlo (RMC) as well as classical molecular dynamics (MD) and Monte Carlo (MC) techniques. MD calculations were conducted in the canonical ensemble, employing an all-atom force-field, while MC simulations were run within the isobaric-isothermal ensemble with a united-atom force-field. RMC simulations relied on X-ray and neutron diffraction data; in addition, partial radial distribution functions (PRDF) from either MD or MC computer simulations were also modeled. We have developed a scheme for classifying hydrogen bonded clusters: aggregates have been divided into 5 distinct types (cyclic branched clusters, acyclic branched clusters, linear chains, isolated rings and isolated composite ring clusters) according to their morphological characteristics. Cyclic structures were found to be an important constitutive part of all of the studied models, with fractions of ring motifs amounting from ~10 % up to ~35 %, depending on the modeling approach, H-bond evaluation scheme and on the size of the alcohol molecule. Ring-shaped molecular aggregates are the most abundant in 1-propanol. It could be conjectured that ring formation is not a completely random process in potential-governed simulations, but instead possesses a certain degree of specificity that differs between isolated rings and rings with peripheral branching.

Neutron and X-ray weighted total scattering structure factors of *liquid chloroform, bromoform and methyl-iodide* ($CHCl_3$, $CHBr_3$ and CH_3I, respectively) have been interpreted by means of RMC modeling. We have focused on a detailed characterization of orientational correlations between tetrahedral molecules of C_{3v} symmetry. These investigations have been complemented by determining dipole-dipole (molecular axes) correlations. Concerning short range correlations (at and just below 4 Å), two neighbouring molecules turn towards each other most frequently according to the 2:3 (edge-to-face) group. In bromoform the occurrence of 1:3 (corner-to-face, or 'Apollo') orientations appear to be significant in a narrow distance range, just below 4 Å. The strongest dipole-dipole correlations also appear at the shortest distances, around and below 4 Å. Among the special molecular axes orientations monitored here, the 'chain-like' arrangements are the most significant.

Borosilicate glasses. — Sodium borosilicate glasses $(75\text{-}x)SiO_2 \cdot xB_2O_3 \cdot 25Na_2O$ with x=5, 10, 15, 20mol% have been prepared by rapid-quench method. The special interest of this ternary system lies in the different glass forming mechanisms of SiO_2 and B_2O_3. One of the main questions is the structural changes of boron-oxygen network and the coordination around B atom induced by the increasing B_2O_3 content. Neutron- and high energy X-ray diffraction experiments have been performed and for data evaluation RMC simulation technique was applied (see Fig. 1 for one of the glasses). A possible 3-dimensional structure model has been obtained which is consistent with the experimental data. Partial atomic correlation functions, coordination number distributions and three-atom bond angle distributions have been revealed. We have established that the basic network is formed by 4-fold coordinated (tetrahedral) SiO_4 units with a first neighbour distance of 1.60 Å. The

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boron surrounding is more complicated, both 3- and 4-fold coordinated oxygen atoms are present. In BO_3 units the first neighbour distance is at 1.40 Å, while in BO_4 units it is at 1.60 Å. The ratio of $BO_3/(BO_3+BO_4)$ numbers is increasing from 20% up to 60% with increasing the B_2O_3 content.

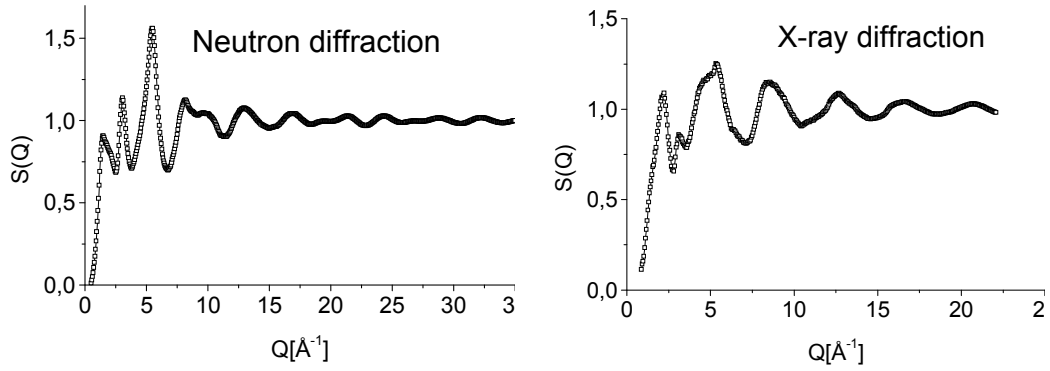

Fig. 1. *Experimental (circle) and RMC (solid line) total structure factors for the $60SiO_2{\cdot}15B_2O_3{\cdot}25Na_2O$ glass.*

Chalcogenide glasses – The structure of amorphous $Ge_{20}Te_{80}$, $Ge_{15}Cu_8Te_{77}$ and $Ge_{15}Cu_5Te_{80}$ has been investigated by diffraction techniques and Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy. In $Ge_{20}Te_{80}$ both Ge and Te obey the 8-N rule and the structure is built up of $GeTe_4$ tetrahedra connected via Te-Te bonding or shared Te atoms connected to two Ge atoms. The coordination number of Te is significantly higher than 2 in glassy $Ge_{15}Cu_8Te_{77}$. In $Ge_{15}Cu_5Te_{80}$ glass, Cu binds mostly to Te, while Cu-Cu bonding is significant in $Ge_{15}Cu_8Te_{77}$. Our findings show that Cu occupies the free space of the host matrix without strongly distorting the network of Ge and Te atoms.

Metallic glasses - The local atomic order of the $Cu_{65}Zr_{35}$ and $Ni_{64}Zr_{36}$ metallic glasses have been investigated in collaboration with IFW Dresden. Large scale models were obtained by fitting simultaneously diffraction and EXAFS measurements by the RMC technique. It is found that there is no essential difference in the partial coordination numbers of the $Cu_{65}Zr_{35}$ and $Ni_{64}Zr_{36}$ metallic glasses, while the mean interatomic distances differ remarkably, especially the Zr-Zr distance which is significantly shorter in the $Cu_{65}Zr_{35}$ glass. Voronoï polyhedra analysis of the RMC atomic configurations reveals that icosahedral atomic ordering is more preferred in the Cu-Zr glass (Figure 2). It is supposed that these features reflect the higher glass forming ability of the $Cu_{65}Zr_{35}$ as compared to the $Ni_{64}Zr_{36}$ alloy.

Yttrium aluminium borate. — $YAl_3(BO_3)_4$ (YAB) single crystals have excellent non-linear optical properties, and doped YAB crystals have important applications in laser engineering. YAB crystals have suitable sites for some rare-earth elements at the Y^{3+} site (Er^{3+}, Nd^{3+}, Yb^{3+}, La^{3+}) or other doping ions at Al^{3+} site (Cr^{3+}, Ga^{3+}). The aim of this study was to investigate the crystallographic effect of the substitution of Er^{3+} and Yb^{3+} into *$YAl_3(BO_3)_4$*. Neutron powder diffraction measurements have been performed on $YAl_3(BO_3)_4$ (YAB), on doped $Y_{0.88}Er_{0.12}Al_3(BO_3)_4$, $Y_{0.5}Er_{0.5}Al_3(BO_3)_4$, $Y_{0.5}Yb_{0.5}Al_3(BO_3)_4$ and on co-doped $Y_{0.84}Er_{0.01}Yb_{0.15}Al_3(BO_3)_4$ (see Figure 3) compositions. It was established that doped compounds are isostructural to YAB. The neutron diffraction pattern has been refined in space group *R*32 using the triple hexagonal Wyckoff notation. Both Er^{3+} and

Yb^{3+} ions occupy the Y^{3+} (3a) sites and not the Al^{3+} (9d) sites. Lattice parameters are decreasing with the increasing amount of dopant elements.

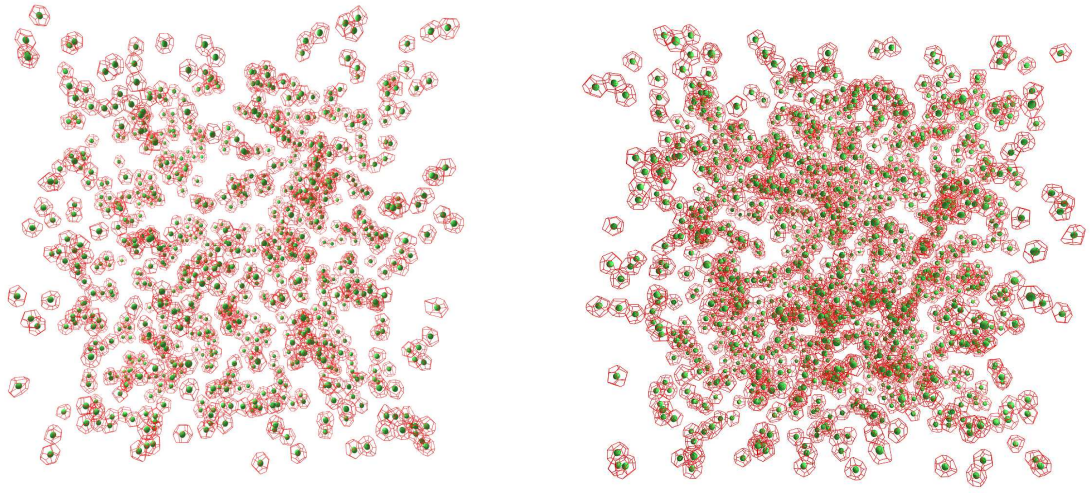

Fig. 2. *Networks of ideal icosahedra in the RMC model configurations for the $Ni_{64}Zr_{36}$ (left panel) and $Cu_{65}Zr_{35}$ (right panel) metallic glasses*

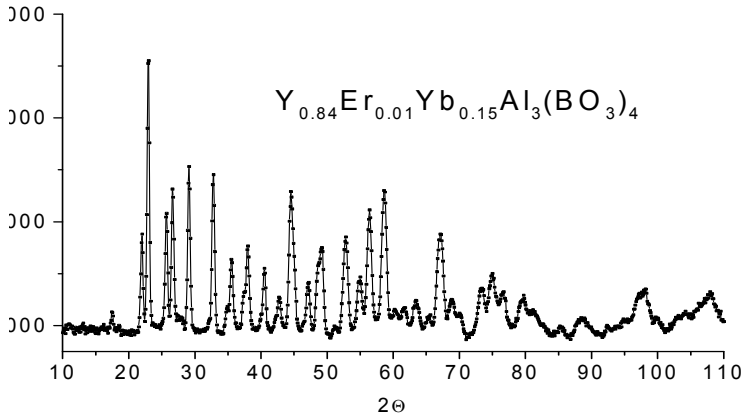

Fig. 3. *Neutron diffraction pattern (λ_0=1.07Å) of $Y_{0.84}Er_{0.01}Yb_{0.15}Al_3(BO_3)_4$*

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Grants and international cooperations

OTKA K083529 Investigations concerning the structure of complex liquids (L. Pusztai, 2011-2014)

HAS-BAS (Hungarian-Bulgarian bilateral) Structure studies of crystalline and amorphous materials by neutron diffraction (E. Sváb, 2010-2012)

HAS-BAS (Hungarian-Bulgarian bilateral) Investigation of disordered materials based on Se-Te chalcogenide glasses by means of neutron diffraction and IR spectrophotometry (E. Sváb, 2010-2012)

TéT SI-06/2009 (Hungarian-Slovenian bilateral) Structural studies of complex liquids (L. Pusztai, 2010-2011)

Long term visitors

— A. Vrhovšek, University of Ljubljana, Slovenia (1 September – 30 November 2011, host: L. Pusztai)

— L. Hawelek, University of Silesia, Katowice, Poland (16 October – 13 November, host: L. Pusztai)

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See also: J.30.

L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, P. Dombi, J. Fekete, Ph. Heck, N. Kroó, P. Rácz, S. Varró

Experimental research. — We carried out experimental investigations on surface plasmon enhanced electron acceleration with few-cycle, carrier-envelope phase (CEP) stabilized laser pulses. We determined the spectrum of electrons accelerated in the plasmonic field and found that signatures of the phase stabilized optical waveform driving the individual electron trajectories are washed out in the electron spectra. We attribute this effect to nanoscale surface roughness of the metallic samples, as supported by extensive numerical simulations. This finding explains the previously observed, low CEP sensitivity of photoemission processes from metallic films and enables the development of femtosecond electron sources for ultrafast time-resolved applications.

We also investigated surface plasmon (SP) waves in the junction of a scanning tunneling microscope (STM). The SP waves were generated on a 45-nm thin Au film and their near-field was locally probed by the tip of the STM. The temporal structure of the observed tunneling current signal revealed information on the physical mechanisms which regulate the interaction of the electric fields in play. We estimated the magnitude of the local electric field enhancement on surface nanostructures by taking advantage of the nonlinearity of the tunneling junction. The mapping of the plasmon field to the surface topography delivers experimental evidence for the localization of SP waves in narrow gaps of a few nanometers width and/or at grain boundaries. Results gained can be utilized directly (e.g., in the development of nanoscale geometries for high-energy electron sources where electrons are accelerated in the electric field of surface plasmons).

We also took part in experiments related to the diffraction efficiency of gratings etched into fused silica. Diffraction efficiency of gratings fabricated with the use of two-beam interferometric laser-induced backside wet etching (TWIN-LIBWE) was successfully modelled.

We continued the investigation of the characteristics of surface plasmons by scanning tunnel microscope. We found that plasmon signal appears on the microscope even in the case when the applied voltage on it is zero – on those areas, where giant fields formed due to the localisation of plasmons (Fig. 1). The signal does not disappear even in the case, when the intensity of the laser light, which excites plasmons, is decreased and extrapolated to zero value. We had to decide between two possibilities. One is the Casimir effect, which has to be independent of the polarity of the voltage applied to the microscope, the other is the multiple charge reflection, which does depend of it. In the course of scanning, when the bias voltage of the microscope was changed from negative to positive direction, and subsequently from positive to negative direction, we observed a certain hysteresis in the plasmon-induced STM-current value (Fig. 2), which fact excludes the Casimir-effect and makes probable the second imagination.

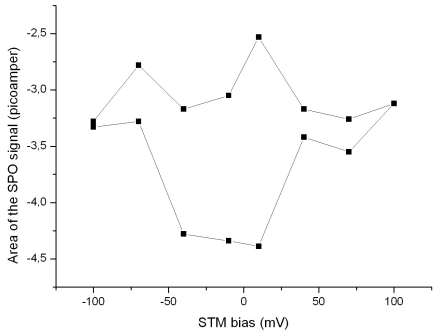

Fig. 1. *Plasmon signal on STM microscope*

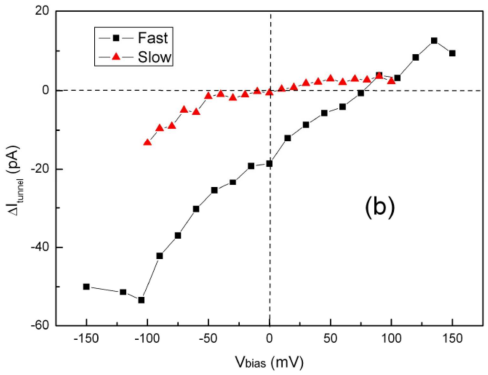

Fig. 2. *Hysteresis in the plasmon-induced STM-current value*

Theoretical research. — High-order harmonic generation by few-cycle 800 nm laser pulses in neon gas in the presence of a strong terahertz (THz) field was investigated (Fig. 3) numerically with propagation effects taken into account. Our calculations show that the combination of THz fields with up to 12 fs laser pulses can be an effective gating technique to generate single attosecond pulses. We show that in the presence of strong THz field only a single attosecond burst can be phase matched, whereas radiation emitted during other half cycles disappears during propagation. The cutoff is extended and a wide supercontinuum appears in the near-field spectra, extending the available spectral width for isolated attosecond pulse generation from 23 to 93 eV. We demonstrate that phase-matching effects are responsible for the generation of isolated attosecond pulses, even in conditions when single-atom response yields an attosecond pulse train.

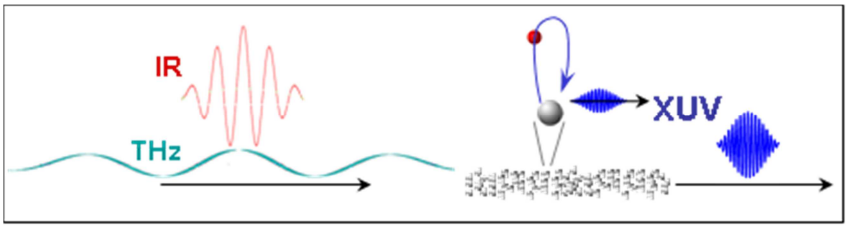

Fig. 3. *Scheme of THZ assisted generation of high order harmonics enabling shorter attosecond pulses*

By investigating nonlinear surface-plasmon-mediated electron emission, a platoless energy distribution was found, when the pulse duration of the exciting laser was comparable with the life-time of surface plasmon oscillations (SPOs). The appearance of large-energy electrons cannot be explained with standard non-perturbative theories, even if one takes into account the field enhancement due to surface plasmons. Experimental results for lower laser intensities are reproduced quite well in our theoretical calculations, both in the low-enegy and in the high-energy part of the spectra. These results firmly support the applicability of our concept of plasmon-induced oscillating near the field of a double layer at the metal-vacuum interface.

We have studied the statistical properties of light emitted by suface plasmon oscillations (SPOs), generated in a gold layer in the Kretschmann geometry, and a detailed analysis of the coherence properties of the SPOs has been carried out. By developing a new formalism for describing the quantum statistical properties of the SPOs as single-photon emitters, the Fano factor and the covariance of counting events, in delayed or spatially separated detectors have been calculated on the basis of the derived analytic formulas. The transition from antibunching to bunching has also been predicted and analysed (Fig. 4), and a reasonable agreement with our new experimental results was achieved.

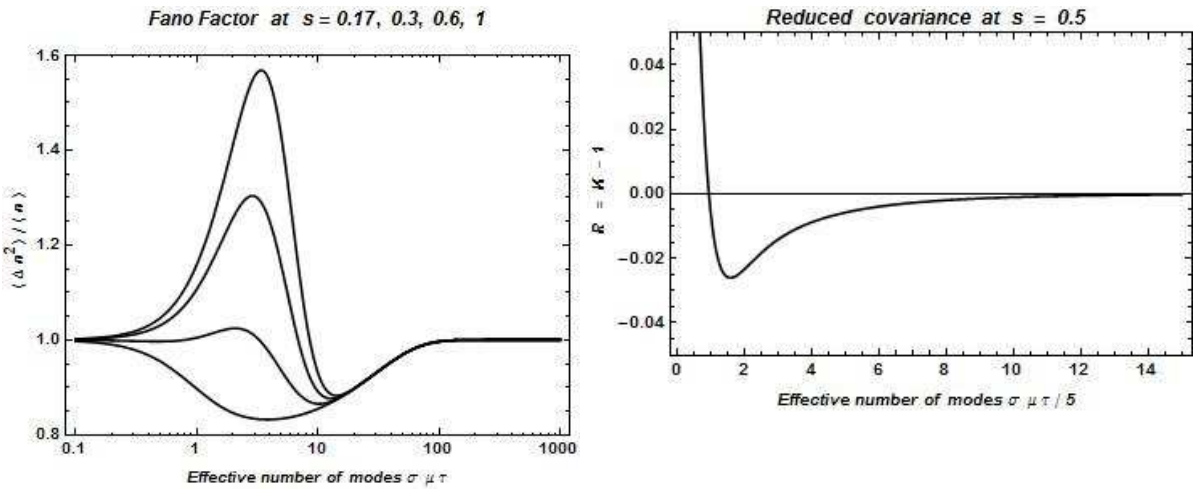

Fig. 4. *Left: shows in a log-linear plot the Fano factor $F = \langle \Delta n^2 \rangle / \langle n \rangle$ on the dimensionless interaction time (which is displayed on the abcissa as „Effective number of modes $\sigma\mu\tau$") for four values of the coupling parameter s (which quantifies the efficiency of coupling of the radiation into the measuring apparatus). The uppermost curve corresponds to the lowest value s =0.17, and lowermost one to the value s = 1. Right: shows the reduced covariance $R = \langle N_1 N_2 \rangle / \langle N_1 \rangle \langle N_2 \rangle - 1$ calculated on the basis of our theory, where $N_{1,2}$ are the numbers of photon countings by the detectors on the opposite sides of the beam splitter. This quantity, like the Fano factor plotted on the left, is very sensitive to the value of the coupling parameter. This part of the figure shows both bunching and anti-bunching of the photocounts.*

In the context of our theoretical work on extreme light sources, we have investigated in details the characteristics of the synchrotron radiation emitted by ultrarelativistic electrons in the interior of a coaxial cylindrical mirror. This is an unconventional geometrical arrangement, where the "superradiance" may be realized in two dimensions, in the Röntgen regime. The present analysis supports our original physical picture according to which, if the electron meets with its own radiation field emitted earlier in a tangential narrow cone, and reflected back by the mirror, then there is a constructive interference between this retarded self-field and the actually emitted radiation field.

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Grants and international cooperations

OTKA 73728 Attosecond dynamics of matter in ultra-high laser fields with sub-cycle temporal and sub-wavelength, nanometer-scale spatial resolution (S. Varró, G. Farkas 2008-2012)

Max Planck Institute for Quantum Optics (Garching, Germany), Surface plasmon research using STM (N. Kroó), Pulse compression of long-cavity Yb thin disk oscillators (P. Dombi)

University of Alberta, Edmonton, Canada, Surface plasmon enhanced electron acceleration with few-cycle laser pulses (P. Dombi)

Institute for Photonic Sciences, Barcelona, Plasmonic electron acceleration experiments with mid-infrared lasers (P. Dombi, P. Rácz)

University of Graz, Investigation of femtosecond photoemission from nanostructures (P. Dombi)

TéT ES7/2008 Ultrafast laser-solid interaction dynamics in the field of intense, few-cycle laser pulses (P. Dombi, P. Rácz, J. Fekete, 2009-2012)

Institut für Quantenphysik and Institute für Quantenoptik, University of Ulm (Ulm, Germany), Quantum optics in phase space. Surface plasmon research. (S. Varró, N. Kroó)

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M. LASER PHYSICS

P. Hartmann, A. Derzsi, Z. Donkó, Z. Gy. Horváth, I. Korolov, A.-Zs. Kovács[#], K. Kutasi, P. Mezei, K. Rózsa, J. Schulze

Gas discharge physics. — In a fruitful collaboration with the Institute for Plasma and Atomic Physics of Ruhr University, Bochum (Germany), we have carried out a series of simulation studies based on the Particle in Cell (PIC) technique. We focused our attention on the power absorption of electrons from radiofrequency electric fields, as well as on the physics of discharges driven by two or more harmonic frequencies. We have as well studied the effect of secondary electrons on the separate control of ion energy and flux in dual-frequency capacitively coupled radio frequency discharges. We developed a simulation code to describe the fast ignition of a hydrogen microdischarge on the nanosecond time scale. The simulation results have been in good agreement with experimental data, concerning the electrical characteristics and the spatio-temporal light emission patterns of the plasma.

In our investigations of radiofrequency discharges operated in electronegative carbon tetrafluoride (CF_4) gas, we found that in contrast to common α- and γ -mode operation, electrons accelerated by a strong electric field in the plasma bulk dominate the ionization. This bulk-mode has been investigated by kinetic particle simulations, experimental phase-resolved optical emission spectroscopy (PROES), and an analytical model. The high electric field in the discharge center was found to be caused by a low bulk conductivity and local maxima of the electron density at the sheath edges. Mode transitions as a function of driving voltage and pressure have been observed.

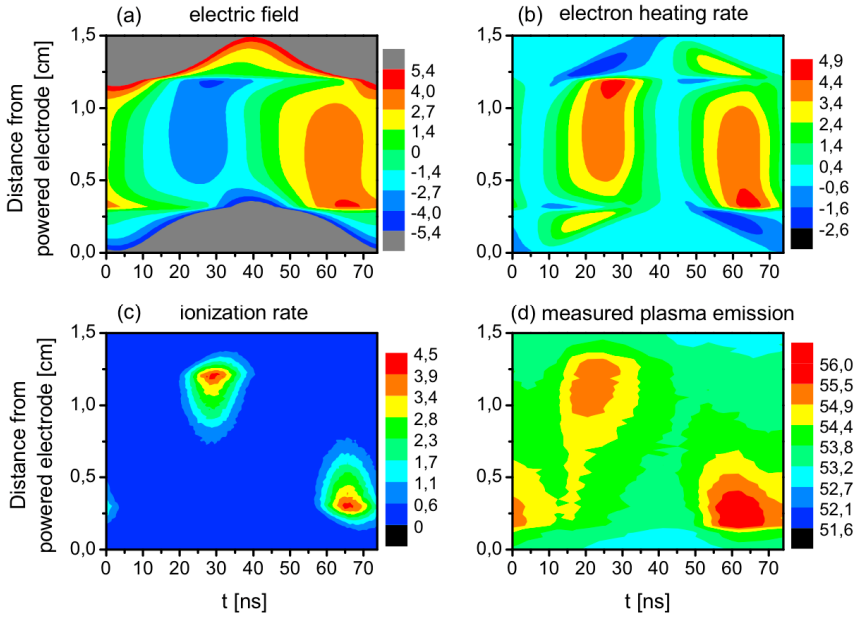

Fig.1. *Spatio-temporal plots of the (a) electric field, (b) electron heating rate and (c) ionization rate obtained from PIC simulation in a CF_4 discharge driven at 13.56 MHz with an electrode gap of 1.5 cm, at 60 Pa and 100 V. The grayscale gradients are given units of 10^3 Vm^{-1} (electric field), 10^4 Wm^{-3} (heating rate) and 10^{21} $m^{-3}s^{-1}$ (ionization rate). (d) shows experimental result (in a. u.): the plasma emission at 250 nm detected space resolved between the electrodes and time resolved within the RF period by PROES.*

We have experimentally investigated the Ar^+-Fe and Ar^+-Ni asymmetric charge transfer (ACT) reactions using a combination of plasma diagnostics methods and a kinetic model

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of the afterglow plasma, which allow monitoring of the temporal evolution of the densities of different species. Metal vapor was created inside a discharge cell by cathode sputtering; its density was measured by atomic absorption spectroscopy. The rate coefficient of the reaction was evaluated from the emission intensity decay of excited and ionized metal spectral lines pumped by the ACT process. In another line of research experimental studies have been carried out to clarify the effect of the anode material on the characteristics of glow discharges used in analytical spectroscopy.

In a multilateral collaboration the electron drift velocity in argon with admixtures of up to 2% of nitrogen, hydrogen or oxygen has been measured in a pulsed Townsend system for reduced electric fields ranging from 0.1 Td to 2.5 Td. The results have been compared with those obtained by Monte Carlo simulations and from the solution of the electron Boltzmann equation using two different solution techniques.

Strongly coupled plasma research. — Molecular dynamics simulations and lattice summation algorithms for binary Yukawa systems (consisting of equally charged, light and heavy particles) were developed. Extensive studies on the longitudinal and transverse acoustic mode phase velocities (sound speeds) revealed that in contrast to the weakly coupled situation, it is the mass of the heavy component that dominates the oscillations in the systems, and thus the sound speed, in agreement with the predictions of quasi-localized charge approximation (QCLA) theory. Extending our investigations to full wave dispersion properties, including all inter-species optic excitations, we have shown the appearance of a mass-ratio invariant mode, and prepared parameter maps of regions of stability of the predicted ground state crystalline structure vs. charge ratio and coupling strength (temperature). In our dusty plasma experiments we have focused our activities on the rheology of two-dimensional systems. We have shown that a single layer dusty plasma in strongly coupled regime exhibits a strong non-Newtonian static shear viscosity (shear thinning) and a non-monotonic frequency dependent complex viscosity covering both the dissipative (viscous) regime at small frequencies and the transition to the elastic regime at high frequencies. Non-equilibrium molecular dynamics simulations support and complement our experimental findings.

Surface wave microwave discharge systems for biomedicine and nanostructuring. — Surfatron generated surface wave microwave discharges created in small diameter tubes contain high density of active species. When discharge is created in flowing gas the active species can be transported into reactors of different size and configuration. It can be used for different applications, such as sterilization of medical tools, deposition of oxide films or oxide nanowires. By means of modeling we have investigated the creation of different species in Ar-O_2 microwave discharges and the evolution of species densities in the afterglow (region downstream the discharge) as a function of different parameters. Special attention has been given to the most extensively used oxygen atoms determining the dissociation degree of oxygen molecules in a wide range of pressure and mixture composition. The surface wave microwave discharge and the small volume afterglow are described by a zero-dimensional kinetic model, while the density distributions in a large volume post-discharge reactor are determined with a 3-D hydrodynamic model.

Electrolyte cathode atmospheric pressure glow discharge (ELCAD). — In order to clarify the very confused T_G gas temperature and n_e electron density data published for ELCAD, the relation between T_G and n_e was studied. In our experiments, T_G was found to be very close to T_e electron temperature indicating that the investigated system is very close in a thermodynamic equilibrium state. Therefore, the values of T_G and n_e can be obtained from the Saha-equation. Saha-equation is mainly valid for highly ionized plasmas

having high charge densities. But the ionization rate of the glow discharges, thus their charge densities are very low. It was numerically demonstrated, that in the case of glow discharges, instead of the Saha-equation, the Engel-Brown approximation could be applied for determining the corresponding values of T_G and n_e. Using this approximation, all T_G and n_e data published together for the ELCAD have been evaluated. Our T_G and n_e data agree with this approximation excellently. Unfortunately, this was not the case for all other data, since incorrect methods were used for T_G determination and the n_e values were stemming from very inaccurate measurements.

Imaging ellipsometer. — The first expanded beam macroimaging ellipsometer was successfully installed at Toledo University (Ohio, USA) as a standard tool on the experimental production line of the Wright Center for Photovoltaics Innovation and Commercialization. Our new method — developed in cooperation with the Research Institute for Technical Physics, H.A.S. — can easily be tested there, by leading experts of the US semiconductor industry.

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Grants and international cooperations

OTKA K 77653 High performance modeling and simulation of low-temperature and strongly coupled plasmas (Z. Donkó, 2009–2013)

OTKA PD 75113 Phase transition and collective dynamics of two-dimensional many-particle systems (P. Hartmann, 2009–2011)

OTKA K 68390 Investigations of atomization processes in an electrolyte cathode atmospheric glow discharge (P. Mezei, 2007-2012)

EU-FP6-MRTN-CT-2006-035459 GLADNET: Analytical Glow Discharge Network (Z. Donkó, 2007-2011)

HAS-SASA Serbian-Hungarian Bilateral Academic cooperation Hybrid models for gas breakdown and formation of plasmas (K. Kutasi 2010-2013)

TéT_10-1-2011-0717 (Hungarian-French bilateral) Study of Ar-O_2 surface-wave microwave discharges and their pos-discharges (K. Kutasi 2011-2012)

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N. LASER APPLICATION

A. Czitrovszky, L. Himics[#], P. Jani, A. Kerekes[#], Á. Kiss, M. Koós, A. Nagy, D. Oszetzky, S. Tóth, L. Vámos, M. Veres

Optical measuring techniques. — The Laser Application Department in co-operation with the Research Institute for Particle and Nuclear Physics HAS, the Optilab Ltd, the Technical University of Budapest and the Research Institute of Atomic Energy, HAS successfully applied for the grant of the National Development Agency, entitled "Establishing of the Budapest Research Centre for ELI Laser Technology" ELI_09-1-2010-0010. Within the framework of the project development of laser technologies, new optical coatings and measurement methods related to *ELI ALPS (Extreme Light Infrastructure Attosecond Light Pulse Source)* have been continued with concentrated efforts. One of the main goals of this project is the development of a 35 fs laser system with 1 kHz repetition rate and 1 mJ pulse energy for high harmonic generation with attosecond pulses and femtosecond optical damage threshold testing. The next task is the elaboration of new optical coating technologies and special optical layers for the utilization in different components of the ELI ALPS (laser mirrors, beam splitters, special filters, etc.). Another aim is the development of interferometric measurement methods for surface diagnostics, alignment control and vibration analysis. Further goals include the elaboration of high dynamic range light scattering techniques for controlling purity of substrates and optical materials.

Airborne particle counters, developed previously, will be utilized for monitoring in clean room setting at several ELI sites.

Portable industrial version of the *dual wavelength optical particle analyzer* (DWOPS), developed earlier, enables the simultaneous measurement of the concentration, size distribution, refractive index and absorption of the aerosol particles. During the environmental disaster in Devecser and Kolontár last year, we used the mobile lab of our department and other instrumentation for measurements at hot spots of the red mud stricken area. During measurement campaigns we collected samples for laboratory analysis with the purpose of studying morphology, Raman spectra, luminescence, etc. Using these methods we discovered several new properties of the air contamination from red mud dusting.

In co-operation with the Research Institute for Atomic Energy, HAS we elaborated computer simulations of airway deposition of intact and fragmented pollens in human respiratory tracks and determined deposition parameters for other different types of contaminations.

A pulmonary waveform generator for in vitro testing and measurement of aerosol flow in transparent hollow human respiratory track models was designed and constructed. Computer controlled pneumatic system enables the generation of any breathing waveform with different air flow parameters. This system is connected to a hermetic transparent chamber holding different lung models and enabling optical measurements using *Laser Doppler Velocimetry* (LDV). A new, compact version of LDV system was also developed. This complex system is planned to be utilized for the verification of the numerical stochastic lung models in order to obtain valuable information on aerosol drug or contamination deposition in different generations within the human lung.

[#] Ph.D. student

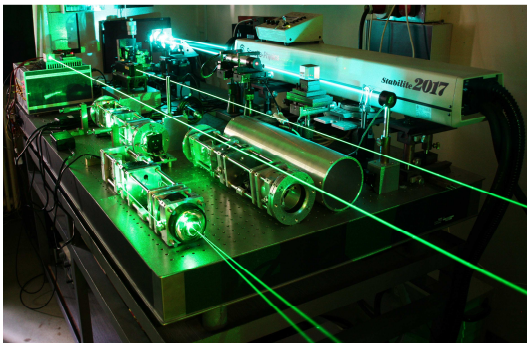

Fig. 1. *The elaborated Nano-LDA photon correlation system*

The activity was fully concentrated on the construction of 2 pieces of serial product *Nano-LDA* photon correlation systems (Fig. 1), within the KMOP-1.1.1-07/1-2008-0056 project and the contract Gi3989/2008 between Technoorg Ltd. - RISSPO.

Prototype testing, calibration and implementation of the opto-mechanical units were completed together with the measurement data collection hardware and software.

Calibration measurements on different particles in the 100–400 nm range were carried out and reported. The online, simultaneous velocity, size and concentration data obtained from single particle transit corresponded to the input data correctly.

The project has passed the inquiry of the control commission and obtained a successful termination report.

Via different FP7 projects we contributed to a series of measurement campaigns organized in many countries of Europe from Portugal to Estonia.

We continued *studying surface plasmon statistics* and increased the time resolution of the measurement system based on cross-correlation function analysis. Using this technique the statistics of light generated by the different non-linear processes, were determined. The great advantage of this method is the independence from the intensity fluctuations of the incident excitation light.

Amorphous carbon layers. — Different forms of nanocrystalline carbon have gave stimulus to basic research and development aiming both understanding of fundamental physical properties and exploiting valuable possibilities with respect to practical applications. Diamond's outstanding properties drew interest of researchers over decades. Nano- and ultranano-crystalline diamond (NCD and UNCD) possessing a wide range of favourable characteristics enhanced intensive research in the last ten years. Due to their large scale synthesis, small primary particle size, outstanding biocompatibility, non-toxicity, surface functionalization as well as stable photoluminescence (PL), nanodiamonds have more advantages in bioapplications than any other nanoparticles. PL in nanodiamonds, originating from structural defects and impurities (dopants), has high quantum yield, without photoluminescence blinking and little photobleaching.

Nitrogen related defect centres in nanodiamonds represent particular importance. Because of promising biological and quantum optical application the NV^- (substitutional nitrogen atom and vacancy) complex centre is the most studied colour centre in nanodiamonds. The utilization of this material, however, requires further efforts in controlling surface properties of nanoparticles and creating new colour centres, which will broaden the scope of applications too.

Our research in the field of nanocrystalline diamond was aimed at studying characteristics of some colour centres formed in the nanoparticles as well as developing simple and effective surface treatment technologies.

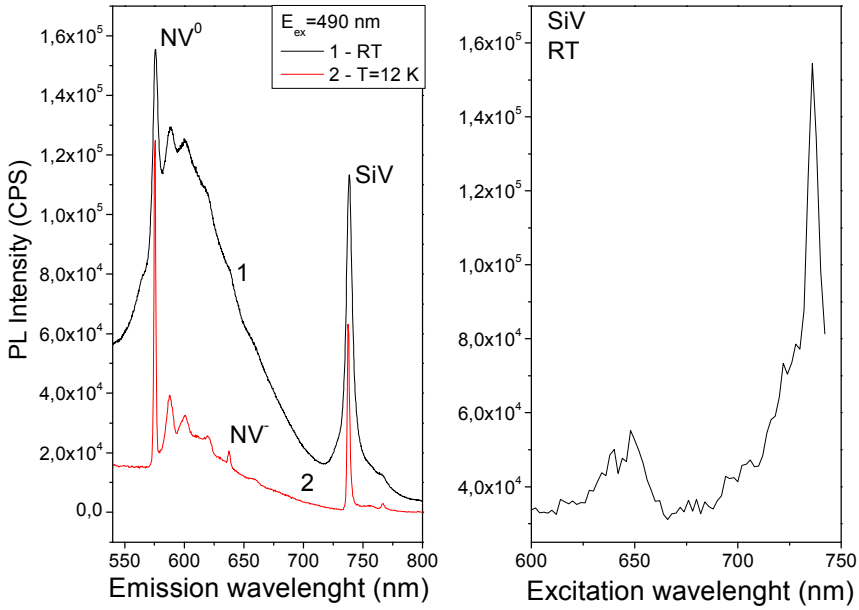

Fig. 2. *Fluorescence and excitation spectrum of SiV centre. Light emission of NV^- and NV^0 centres are also observable.*

In collaboration with a Russian research group we started to investigate nanodiamonds containing silicon-vacancy complex (SiV) centres prepared by microwave chemical vapour deposition (MWCVD) method. Silicon-vacancy complex as a single photon source shows a sharp zero phonon line (ZPL) at 738nm (1.68 eV) in the PL spectrum and exhibits only very weak vibronic sidebands at room temperature. SiV centers can be excited in photon energy region transparent in living tissues, so they have very promising biological applications. Fig.2. shows the emission and excitation spectra of SiV complex measured at room temperature. Intensive narrow band of emitted light exhibits no photobleaching even after laser excitation for several days. These samples contain NV^- and NV^0 colour centres, too, which allow tuning of the emission wavelength. The lateral distribution of SiV fluorescence intensity measured with 1 micron excitation spot diameter using a microscope is shown in Fig.3. In the near future our scientific challenge is to create one photon emitting nanodiamonds from these microcrystals.

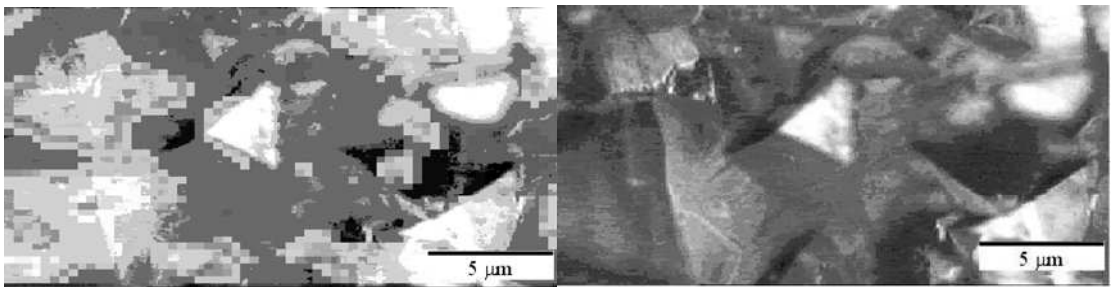

Fig. 3. *Distribution of the 738 nm SiV PL peak intensity (left) on MWCVD microcrystalline diamond and the optical image of the relevant area. The step size was 200 nm. Black means the lowest and white is the highest intensity.*

Implantation with nitrogen ions and bombardment with energetic (typically 2 MeV) particles to introduce intrinsic defect centres are the most frequently used methods for preparation of fluorescent nanodiamond. Plasma immersion ion implantation (PIII) and fast atom beam (FAB) treatments can be considered as cost effective and simple alternatives.

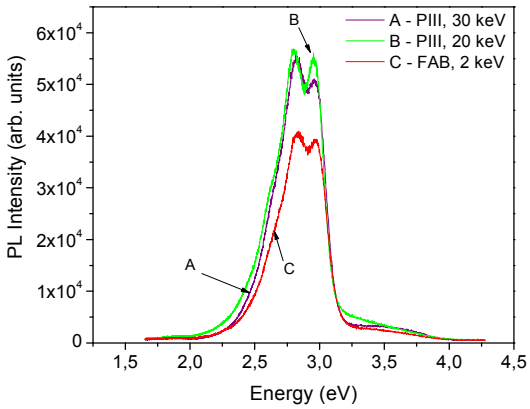

Fig. 4. *Fluorescence spectra of N3 centres in 20 nm nanodiamond particles irradiated with He^+ and N^+ ions of different energy.*

Therefore we have started to investigate defect centres produced by PIII and FAB techniques in nanodiamond with sizes below 20 nm. He^+ ions and N^+ ions of 2, 20, 30 keV energy with different ion fluxes have been used for intrinsic and extrinsic defect generation, respectively. This was followed by high temperature (800 ºC) thermal treatment in vacuum or inert gas in order to induce migration of carbon vacancy to nitrogen dopant. Fluorescence measurements indicate the formation of N3 centres having zero phonon line at 2.985 eV (415 nm) in studied samples. In Fig.4 the emission spectra containing phonon side band due to N3 centres are shown for nanodiamonds treated by PIII and FAB methods. N3 centre, being a complex one, is formed by 3 substitutional nitrogen atoms and a carbon vacancy. This centre is paramagnetic, so electron spin resonance measurements are under way for an additional confirmation. Stark shift of N3 fluorescence band in natural diamond offers promising application of the material in biolabeling.

Exploitation of the application potential of nanodiamond strongly depends on cleaning and stabilization of nanoparticle surface. Instead of prevailing chemical methods we have started to utilise thermal and plasma treatment. The effectiveness of the procedure was monitored by the changes in the Raman and fluorescence spectra. It was found that both the sp^2 carbon content and clustering of C atoms change remarkably following the heat treatment in oxidative environment at 430-450 ºC. Therefore, this method is able to eliminate the disadvantageous gap states of sp^2 carbons. Nanoparticle surface was altered also by hydrogen and water plasma treatment. Hydroxide groups were formed effectively in water plasma. Further promising studies in this field are under way.

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Grants and international cooperations

0217/2007/OM Jedlik Ányos Programme, Contribution to the fulfillment of the requirements set in the new EU directives with relation to measuring and decreasing the aerosol pollution in the atmosphere (A. Czitrovszky, 2007-2011, 0217/2007 SZFKI-HAS Support for the grant No 0217/2007/OM)

212105/ELI EU FP7 ESFRI, Extreme Light Infrastructure, co-ordination of Hungarian participants (A. Czitrovszky, 2007-2011)

ELI_09-1-2010-0010 NFÜ Establishing of the Budapest Research Centre for ELI Laser Technology (A. Czitrovszky, 2010-2013)

KMOP-1.1.1-07/1-2008-0056, Development of non-invasive nano-particle measurement system (P. Jani, 2009-2011)

IAEA-15455 Porous polymer drug-eluting coating prepared by radiation induced polymerization (M. Veres, 2010-2011)

Gi3989/2008 Technoorg-Linda Ltd. - SZFKI, Development of nano-LDA system, (P. Jani, 2009-2012)

HOYA-SZFKI Contract, Measurement and analysis of air pollution in Mátészalka HOYA corporation (A. Czitrovszky, 2010- 2011)

410/EAC EAC Conference (A. Czitrovszky, 2011)

TÉT KR-6/2009 Hungarian Korean bilateral Intergovernmental cooperation. Surface modification of nanodiamond by conductive polymer (M. Veres, 2010-2012)

HAS-RAS Hungarian Russian Academic co-operation (M. Veres, 2011-2012)

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N.9. Lukács* R, Veres M, Shimakawa* K, Kugler* S; Photoinduced bond breaking in a-Se: Raman spectroscopic study; *physica status solidi (c);* **8**, 2789–2791, 2011

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See also: L.7., L.15.

O. FEMTOSECOND LASERS

R. Szipőcs, P. Antal[#], D. Csáti, A. Kolonics, Z. Várallyay

Last year, two new laboratories were built for our research: one for novel femtosecond fiber laser technologies and one for development of new nonlinear microscopic techniques for 3D biomedical imaging. In the former, we are focusing on research and development of femtosecond pulse Yb-fiber lasers, amplifiers and application of newly developed photonic crystal fibers (PCF-s), and photonic bandgap (PBG) fibers for dispersion compensation (hollow core fibers) and nonlinear wavelength conversion (solid core fibers). In the latter, we test and develop new nonlinear 3D imaging techniques, such as multi-photon absorption fluorescence microscopy, second harmonic generation (SHG) microscopy and coherent anti-Stokes Raman Scattering (CARS) microscopy using our new, commercial Axio Examiner LSM 7 MP laser scanning microscope (product of Carl Zeiss).

Nonlinear 3D microscopy has the main advantage of imaging deeply in a biological sample with minimum perturbation or damage in the tissue. This technique also has the potential for high spatial resolution, in vivo 3D tomography of the human skin at depths down to 200-500 μm. Its application for melanoma detection diagnostics, cosmetic research, skin aging measurements and drug monitoring has already been demonstrated. Optical disease diagnosis can be enhanced in sensitivity by the application of exogenous fluorescent labels to obtain molecularly specific information from the tissue, but these are typically toxic. Intrinsic fluorophores, such as elastin, melanin, flavines and reduced nicotinamide adenine dinucleotide (NADH), are naturally part of the skin and can be used for imaging. Second harmonic generation (SHG) can be induced to detect the collagen network for instance. Coherent anti-Stokes Raman scattering (CARS) allow for label-free imaging of tissue with chemical contrast and high spatial and temporal resolution. In CARS, laser beams at two frequencies, called the pump, ω_p, and Stokes, ω_S, frequencies are used to illuminate the sample. When the difference frequency between the two beams is tuned to match an intrinsic molecular vibrational frequency in the sample, ω_{vib}, a nonlinear interaction occurs: new light is generated at the anti-Stokes frequency, $\omega_{as} = 2\omega_p - \omega_S$, by the CARS process. CARS imaging offers chemical selectivity, high spatial resolution imaging in vivo in living animals and humans.

For single wavelength nonlinear microscopy, typically broadly tunable, femtosecond pulse Ti-sapphire lasers are used. This year we developed a simple wavelength extension unit for these tunable lasers comprising a two stage Yb-fiber amplifier unit, which allows CARS measurements practically on the same microscope and laser-setup that is used for single wavelength 3D microscopic imaging. In the following, we briefly introduce this novel two wavelength, inherently sysnchronized laser system suitable for label free, CARS microscopy. The experimental setup is shown in Fig. 1. A broadly tunable, femtosecond pulse Ti-sapphire laser (FemtoRose 100TUN NoTouch, product of R&D Ultrafast Lasers Ltd.) generates nearly transform limited, τ_{FWHM} ~190 fs pulses for our measurements. A beam-splitter (BS) divides the laser power into two parts: the reflected beam is focused into a small core area photonic crystal fiber by a high NA, aspheric focusing lens, which generates the seed pulses for the two-stage Yb-amplifier unit (FemtoFiber, product of R&D Ultrafast Lasers Ltd.) operating at around 1030 nm. The transmitted beam, which plays the role of a tunable pump beam for CARS measurements, directly goes into

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nonlinear microscope passing through a precision delay stage, which assures the zero delay difference between the tunable pump and amplified, compressed Stokes pulses, the latter one is being generated by the two-stage Yb-amplifier unit. The pump and Stokes pulses are inherently synchronized, since the seed pulses of the amplifier are generated by the Ti:sapphire laser pulses by efficient nonlinear wavelength conversion in the photonic crystal fiber (PCF).

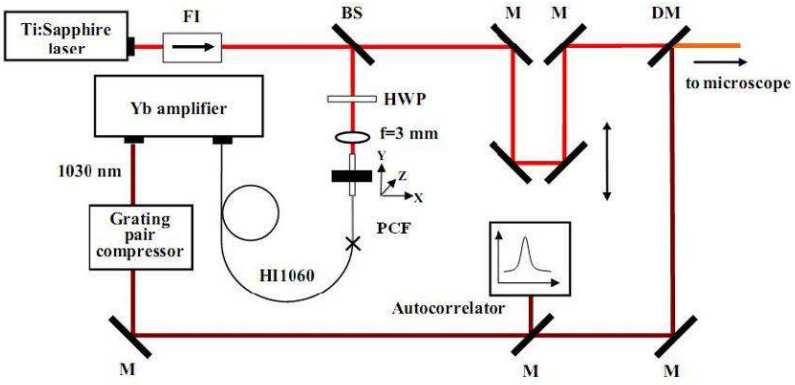

Fig. 1. *Setup of the CARS extension unit*

For seeding the Yb-amplifier, we use that portion of the optical spectra of the continuum generated in the PCF, which are within the gain bandwidth (~ 1020-1080 nm) of the amplifier. In Fig. 2, the spectral intensity vs. wavelength functions, which were measured directly after the PCF, are plotted for different pump wavelengths at coupled power levels of ~ 100 mW.

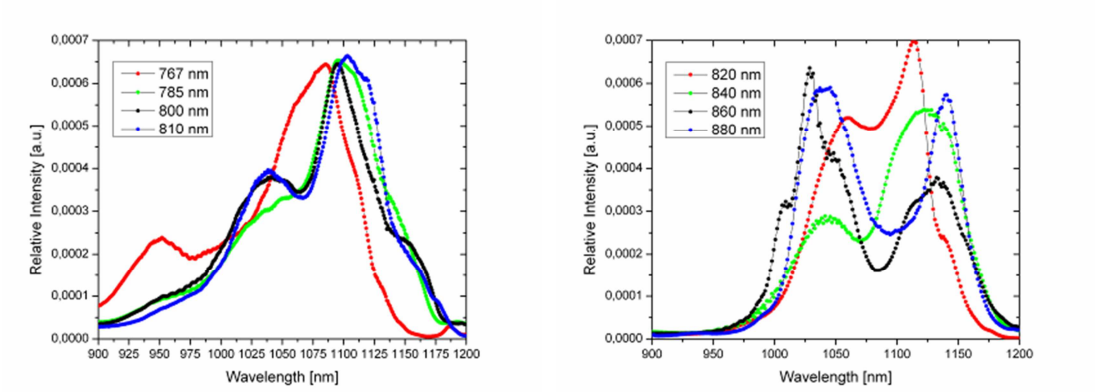

Fig. 2. *Measured spectral intensity distributions of the continuum pulses exiting the PCF at coupled power levels of ~100 mW*

After the two-stage Yb-amplifier, we obtain optical pulses with central wavelength of ~ 1030 nm and a FWHM bandwidth of 11 nm. Using a transmission grating pair compressor, we get nearly transform limited pulses with duration of ~276 fs. The pump and the Stokes beams are combined by a dichroic beamsplitter (DM), and then transmitted to the nonlinear microscope. Both the pump and the Stokes laser provide nearly transform limited optical pulses, hence we expect a relatively strong anti-Stokes signal in our nonlinear microscope. The dual wavelength, inherently synchronized laser system has been tested for label-free, coherent anti-Stokes Raman scattering (CARS) imaging in the Axio Examiner LSM 7 MP microscope. Different samples including mouse dorsal skin, muscle tissues and carbon nanotubes were used for testing. In Fig. 3, we show a CARS image recorded for a carbon nanotube sample deposited to an optical glass substrate.

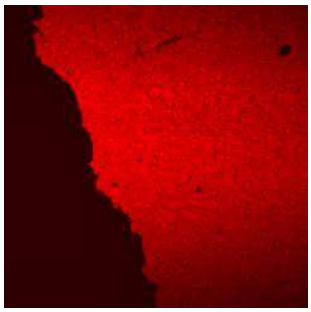

Fig. 3. *Images taken by nonlinear microscopy. CARS image of carbon nanotubes deposited onto an optical glass substrate*

According to Raman spectroscopy measurements, the sample has a strong vibration resonance at ω_{vib} = 2577 cm^{-1}. For the CARS measurements, the pump laser had to be tuned to 814 nm (12285 cm^{-1}) in order to satisfy the $\omega_{vib} = \omega_p - \omega_S$ condition. Since the Stoke beam is centered at 1030 nm (9708 cm^{-1}), the anti-Stokes signal should be detected on the "red" channel of our nonlinear microscope at the wavelength of 673 nm.

Based on our measurements, we are convinced that this novel, simple, cost efficient, inherently synchronized Yb-fiber laser based extension unit introduced here is well suited for upgrading most of the existing single wavelength nonlinear microscope setups for dual wavelength, label-free, coherent anti-Stokes Raman scattering imaging.

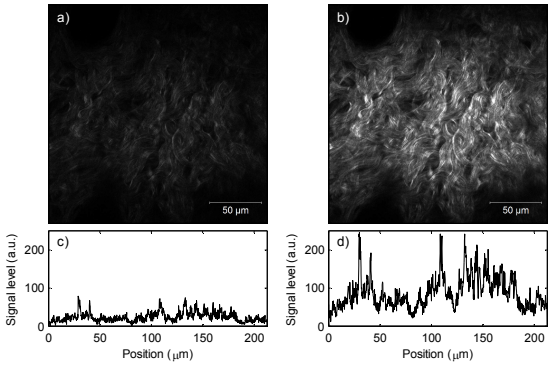

Fig. 4. *Images taken by nonlinear microscopy. Two-photon absorption fluorescence images of mouse dorsal skin using (a) the 76 MHz laser and (b) the 22 MHz laser, at nearly the same excitation power (3.081 mW for the 76 MHz laser and 3.015 mW for the 22 MHz laser). (c) and (d) show the corresponding intensity profiles for the horizontal line in the middle of the images.*

Taking the advantage of our new nonlinear microscope, we have also tested our broadly tunable, long-cavity, low-pump-threshold, pulsed Ti:Sapphire laser for biomedical imaging. This novel laser system has been introduced briefly in the previous issue of this Annual Report. The laser delivers nearly transform limited ~140 fs, ~10 nJ pulses at 19.6 MHz repetition rate using a 2.5 W green pump laser source. These features result in a higher signal to noise ratio, a lower photo-degradation of biological samples. Furthermore, it is a more cost efficient construction than its 80 MHz predecessors, and hence this laser construction is ideal for nonlinear microscopy applications. This fact is demonstrated in Fig. 4, where two-photon absorption fluorescence images of mouse dorsal skin using (a) the 76 MHz laser and (b) the novel 22 MHz laser are shown, using the same excitation average power.

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Grants and international cooperations

OTKA K-75404 Design and application of photonic crystal fibers for femtosecond pulse optical fiber lasers, laser amplifiers and optical parametric oscillators (R. Szipőcs, 2009-2012)

TECH-09-A2-2009-0134 National Technology Program, Development of fiber integrated nonlinear microendoscope for pharmacological and diagnostic

examinations based on novel fiber laser technology (Coordinator: R. Szipőcs, 2009-2012)

ELI_09-1-2010-0010 NFÜ Establishing of the Budapest Research Centre for ELI Laser Technology (Participant: R. Szipőcs, 2011-2012)

Contract

SZFKI - University of Szeged: Development of nonlinear microscopy for brain imaging (Coordinator: R. Szipőcs, 2011)

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Articles

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O.2. Antal P, Szipőcs R; Relation between group delay, energy storage and loss in dispersive dielectric mirrors*, Chinese Optics Letters*, accepted for publication

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O.3. Szipőcs R, Kolonics A, Antal P; Tunable, low repetition rate, femtosecond pulse Ti:Sapphire laser for in vivo nonlinear microscopy, In: *Intracellular Fluorescence Spectroscopy,* the Satellite Conference of the 8th European Biophysics Congress, Pécs, 20-20 August, 2011, Paper Talk 2, 2011

P. OPTICAL THIN FILMS

K. Ferencz

Optical thin film structures consisting of nanoscale laminated layers. – We have continued our research concerning the development of optical thin film structures containing nanooptically thin layers for advanced applications in laser physics and measurement technology. Using multiple target thin film optimisation method and our electron-beam deposition technology we have developed several new kinds of optical coatings. Some examples:

— wide-band low dispersive antireflection coating for dispersion compensating glass wedges (BK7 glass, size 20 x 50 mm, wedge angle 8°, wavelength range 650 – 1050 nm),

— high damage threshold ultrafast harmonic separator mirrors (HR_s 400 nm & HT_p 800 nm/45°) on superpolished fused silica substrates,

— low dispersive protected Ag-mirrors for the visible spectral range type "M800" (R > 98% in the range 475 – 975 nm at 0° angle of incidence, R > 98% in the range 484 – 900 nm at 45° angle of incidence, peak reflectance approx. 99% at 600 nm wavelength),

— wide-band antireflective coating consisting of 11 layers on fused silica window substrates (type "AR 600_1000_0g"),

— high damage threshold AR 940 nm/0° coating on convex fused silica lens surfaces (Ø25.4 mm, f = +25 mm),

— TiO_2/SiO_2 dielectric resonator mirrors for SBR structures in GaAs wafers,

— low reflectance loss band-filter structure for 532 nm laser wavelength (HBW ≈ 55 nm, T_{max} = 99%).

Our indium-tin-oxide (ITO) layers having prescribed electrical resistance and visible optical transmittance were successfully applied as heatable windows or in integrated optical biological sensors.

Superpolishing technology. – We have further refined our optical superpolishing technology with adding special chemical materials to the polishing slurry for reducing the probability of nanoparticle aggregation. The result of the technological modification is the improved quality of laser mirror substrates (lowest scratch/dig values) and the highest yield of the polishing process.

The above summarized results will have high importance in the production of high quality laser optical elements for femtosecond petawatt laser facilities planned in the framework of the European project ELI.

These achievements are the results of the scientific cooperation between the Institute and Optilab Ltd.

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Contract

OPTILAB-SZFKI No. 198/2011

Grants

OM-00078/2008 R&D of materials and methods, system–integration for neutron research instruments with the aim of introducing new marketable products (Mirr2007)

OM-00202/2008 Advanced environment friendly thin film solar cells (TFSOLAR2)

ELI_09-1-2010-0010 NFÜ Establishing of the Budapest Research Centre for ELI Laser Technology (Participant: K. Ferencz, 2011-2012)

Q. GROWTH AND CHARACTERIZATION OF OPTICAL CRYSTALS

I. Földvári, L. Bencs, E. Beregi, G. Dravecz[#], K. György[#], N. Laczai, Á. Péter, K. Polgár, Zs. Szaller, É. Tichy-Rács[#]

Growth and study of nonlinear borate crystals. — $YAl_3(BO_3)_4$ (YAB) and $GdAl_3(BO_3)_4$ (GAB) single crystals were grown by the top-seeded flux technique (TSSG). The crystal field transitions of Pr^{3+}-ions were analyzed in YAB crystals by high resolution Fourier transform (FT) spectroscopy in the 500-25000 cm^{-1} wave number and 9-300 K temperature ranges. In spite of the complex spectra the entire energy level scheme was determined for 10 excited manifolds ($^3H_5$, $^3H_6$, $^3F_2$, $^3F_3$, $^3F_4$, $^1G_4$, $^1D_2$, $^3P_0$, $^3P_1$+$^1I_6$ and $^3P_2$). The careful analysis of the spectra as a function of the temperature allowed identifying most of the sublevels of the $^3H_4$ ground manifold. The thermally induced line shift was described by a single phonon coupling model. The orientation of the dielectric ellipsoid and of the associated dipole moments were also determined to several transitions from linear dichroism measurements. The experimental data were fitted in the framework of the crystal-field theory with limited agreement, as was shown typical to Pr^{3+}-ions in various other host crystals. The measured splitting for specific levels was explained by local symmetry reduction around the Pr^{3+}-ions.

Summarizing the spectroscopic information from high resolution FT measurements of rare earth (RE) and Cr^{3+} doped YAB crystals, it was possible to monitor cross-contamination in those crystals. The analysis has shown that Cr^{3+}, Nd^{3+} and Yb^{3+} are the most frequent unwanted impurities. This method is non-destructive for the sample, and rather sensitive. The detection limit for Er^{3+} was 10^{-4} mol%. In addition, the valence of the RE ions inside the crystal could easily be identified. Maps of the impurity distribution was obtained by using a microscope, coupled to the FT spectrometer.

Growth and study of scintillator crystals. — Principal refractive indices of $Lu_xY_{2-x}SiO_5$ (LYSO, x=1.6) single crystal were determined at seven wavelengths between 400-700 nm (interval for scintillator applications) using the classical minimum angle deviation method. LYSO was classified as optically positive biaxial crystal, with optical axes crossing angle $2V_z$=22.45°, and the principal refractive indices were n_x=1.8077, n_y= 1.8110 and n_z=1.8307 at λ=524 nm. Angular dispersion of the principal axes (Y, Z) was determined by ellipsometry. Rotation of the extinction angle in (010) plane was about 8° for the range of 250-900 nm, and 2.4° between 400-700 nm. The reliability of measurements permitted to deduce constants of a common dispersion formula, and use for extrapolating the refractive indices with precision of ±0.001 for wavelengths up to 1100 nm (interesting range for laser applications).

$Li_6Y(BO_3)_3$ and $Li_6Gd(BO_3)_3$ were synthesized by a wet-chemical method from stoichiometric amounts of Li_2CO_3 and Y_2O_3 (or Gd_2O_3). The precipitated, dried powders were annealed at different temperatures with intermediate grinding. Phase purity was tested by FTIR, Raman, and X-ray powder diffraction analyses. Accordingly $Li_6Y(BO_3)_3$ / $Li_6Gd(BO_3)_3$ were produced as major phases accompanied by Li_3BO_3, $Li_6B_4O_9$ and YBO_3 impurity phases.

Single crystals of $Li_6Y(BO_3)_3$ have been grown by both the Bridgman and Czochralski methods with a maximum yield of ~ 80 wt%. It was found that the complex nature of the

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melt solidifications affects the efficiency of the crystallization process and the composition of the grown crystals. High supercooling favored melt dissociation and the formation of thermodynamically unstable phases <$Li_3Y(BO_3)_2$> and <$Li_3Y_2(BO_3)_3$>. The room temperature stability region of <$Li_6Y(BO_3)_3$> phase was investigated on melted and air-quenched ceramic samples in the composition range of Y_2O_3: 8-16 mol%, B_2O_3: 27-35 mol% and Li_2O: 57-65 mol%. It was found that the off–stoichiometric $Li_6Y(BO_3)_3$ phase is extended towards the B_2O_3 rich, Y_2O_3 deficient compositions and the off-stoichiometry has increased the cell volumes.

Growth and study of potassium/lithium niobate (KLN) crystals. — The compositional variation of KLN-1 single crystals grown by top-seeded solution growth (TSSG) method was investigated. During the TSSG growth process the Nb_2O_5 segregation coefficient was found to be constant ($k_{sol/liq}(Nb_2O_5)$~1.2). The actual Nb_2O_5 content of KLN crystals depended both on the growth direction and the crystallization temperature, the Nb content was less in <110> pulled than <001>/<100> crystals under the same growth condition. In order to correlate structural and physical properties of the crystals to the $[K^+]/[Li^+]$ cation ratio in the liquid, alkali homologue ions (Na^+, Rb^+ and Cs^+) have been added as dopant. The alkali cation composition (K/Li ratio) and alkali homologue dopant (Na, Rb and Cs) influenced the Nb_2O_5 content via the variation of the crystallization temperature.

Development of analytical methods for materials science and environmental control. —- Doped bismuth tellurite (Bi_2TeO_5) optical crystals were analyzed for their Er and Nd content by energy dispersive X-ray fluorescence spectrometry using matrix-matched standards for calibration. The results are in good agreement with those obtained from former spectrochemical methods.

Tropospheric ozone (O_3) levels were determined at suburban areas in Santa Clara, Cuba by passive diffusive samplers and UV-VIS spectrophotometry. The overall average value was 24 μg/m^3. The O_3 concentration was the highest in the cold season, and it showed site-specific variation. In the warm season, the observed lower O_3 levels were similar for each sampling site. Models, based on Cochrane-Orcutt algorithm, were fitted to the data set of each season to explain the change in the O_3 concentrations under various meteorological conditions.

Atmospheric aerosols (PM_1 and PM_{10-1}) and pollutant gases (O_3, NO_2, SO_2 and NH_3) were studied at the Alhambra monument, in Granada, Spain during summer and winter. Natural PM_{10-1} aerosols, such as carbonate-rich soil and sea salt, reacted with a typical urban atmosphere, producing a mixture of particulates with diverse chemical composition. The content/formation of secondary inorganic aerosols depended on the temperature and humidity. Ratios of typical mineral elements (i.e., Ti-to-Fe and Si-to-Fe) showed that Saharan dust events contribute to the mineral aerosol content. Black carbon, V and Ni originated from diesel exhaust, while Cu, Cr, Pb and Zn came mainly from non-exhaust vehicular emission.

Ion chromatographic methods were optimized for separation of fluoride, acetate and formate. Using Allsep IC SI-50 4E columns detection limits of 0.014, 0.22 and 0.17 mg/l, and precision of 1.7, 3.0 and 2.8 % was achieved for fluoride, acetate and formate, respectively. This column was applied for the determination of airborne acetic and formic acid levels in the Metropolitan Museum of Art, New York. Atmospheric concentrations of acetic and formic acid up to 1050 and 450 μg/m^3, respectively, were found in non-aerated showcases, which pose a damage risk to the cultural heritage items displayed.

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Grants and international cooperations

OTKA K 68390 Investigations of atomization processes in an electrolyte cathode atmospheric glow discharge. (P. Mezei, contributor L. Bencs, K.György, 2007-11)

OTKA CK 80896 Scintillator materials for medical imaging. (L. Kovács, contributors: Á. Péter, K. Polgár, É. Tichy-Rács, N. Laczai, 2010-13)

OTKA K 83390. Resonant optical processes in solids (L. Kovács, contributors: Á. Péter, K. Polgár, Zs. Szaller, 2011-2015)

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HAS-Russian Academy of Sciences program. Growth of single crystals with wide band-gap and investigation of their crystal lattice defects by spectroscopic methods (J. Janszky, K. Polgár, 2011-2013). Partner: Joffe Phys. Techn. Institute, RAS, St. Petersburg.

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See also: R.3., R.8., R.11.

R. CRYSTAL PHYSICS AND NONLINEAR OPTICS

L. Kovács, I. Bányász, G. Corradi, I. Hajdara[#], E. Hartmann, K. Lengyel, L. Malicskó, G. Mandula, A. Watterich

Modelling crystal structure and the location and vibrations of OH^- in $LiNbO_3$. — Using SIESTA software code the structure of congruent $LiNbO_3$ was studied. An approach based on a supercell consisting of 3x3x3 hexagonal unit cells and containing 4 Li vacancies and 1 antisite Nb (Nb located at the Li site), representing a reasonable approximation for the Li/Nb ratio in the congruent crystal, was found to adequately describe the structure of the bulk. Based on our present and earlier experiments and recent calculations, a new absorption band detected at 4009 cm^{-1} in stoichiometric $LiNbO_3$ single crystals has been assigned to a combination transition involving the OH stretching and an OH librational mode. The librational mode participating in this combination is of lower fundamental frequency than that contributing to the combination band at 4415 cm^{-1} observed earlier.

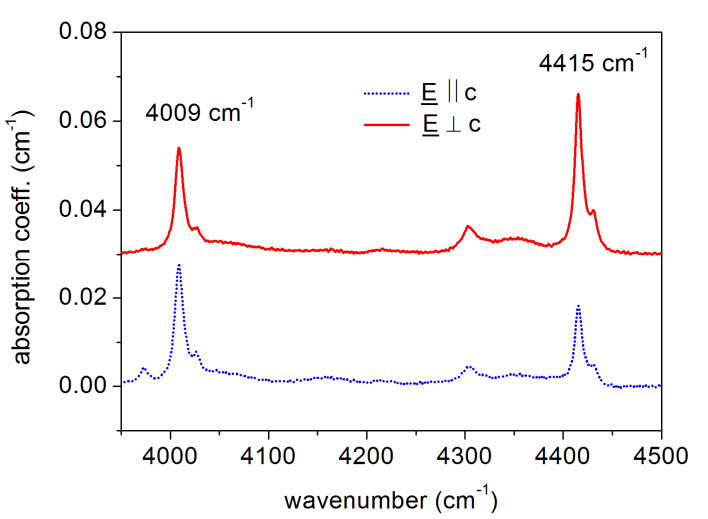

Fig.1. *The IR absorption spectra of a nearly stoichiometric $LiNbO_3$ crystal measured at T = 8 K. The bands at 4009 and 4415 cm-1 are attributed to the stretching + bending combinations of the OH− modes, while the other features may be related to combinations of hydroxyl vibrations with phonons.*

Coherent radiative processes in rare earth doped $LiNbO_3$. — A simple, pulsed pump-probe measurement scheme developed to measure the homogeneous linewidth of an atomic transition in an inhomogeneously broadened spectral line of a dopant ion in a single crystal was applied to the $^2F_{7/2}$ – $^2F_{5/2}$ optical transition of ytterbium in $LiNbO_3$:Yb^{3+} crystals. Using the obtained homogeneous linewidth of about 18 MHz, a dipole relaxation time of ≈ 110 ns has been determined. A population relaxation time of ≈ 0.2 ms has been estimated as well.

Transient absorption of niobate and borate single crystals. — Pump-probe studies of small polarons produced or destroyed by nanosecond laser pulses, with the induced absorption or transparency detected from the nanosecond to the minute range, were used to characterize $LiNbO_3$ single crystal samples of various compositions and dopings, and proved to be a stringent test of the crystal bulk and its quality. In contrast, similar studies on β-barium metaborate (BBO) samples produced using various growth and processing methods showed high sensitivity with respect to surface effects.

Luminescence of Ag and Cu centres in lithium tetraborate single crystals. — Ag co-doping has been shown to significantly enhance the luminescence yield of the tissue-

[#] PhD student

equivalent thermoluminescent dosimeter and neutron detector material $Li_2B_4O_7$:Cu. Part of the absorbed radiation energy is stored in trapped-charge centres which may be stabilized by dopants and other crystal defects. While low temperature spectra of X-ray and cathodoluminescence have the signature of bulk and dopant-assisted excitonic emission, the corresponding higher temperature spectra, depending on the activator dopants present, are due to Cu^+ and/or Ag^+ emission, similarly to those appearing in thermoluminescent dosimeter readout.

Raman spectroscopy of alkali-doped potassium lithium niobate crystals. — Raman spectra have been measured in both pure and alkali (Na, K, Rb, Cs) doped potassium lithium niobate (KLN) crystals. The Raman shift of the A_1(TO) mode belonging to the NbO_6 oxygen octahedral vibration at about 640 cm^{-1} depends only on the Nb content both in pure and alkali homologue doped KLN crystals. The phonon modes at ≈ 306 cm^{-1} and ≈ 350 cm^{-1} corresponding to K^+ and Li^+ ion vibrations, respectively, have been identified by Na doping and ^{6}Li isotope substitution. Raman measurements show that Na^+ ions substitute for both Li^+ and K^+ ions, while Rb^+ ions incorporate only at K^+ sites in the potassium lithium niobate crystal lattice. The incorporation of Cs^+ ions was found to be below the detection limit of Raman site spectroscopy. All these results are in good agreement with the alkali cation vacancy formation model elaborated earlier to describe the charge compensation of Nb_{Li} atoms and the amount of intrinsic defects from concentration data.

Multiferroic materials. — The optical absorption spectra of hexagonal rare-earth manganites ($RMnO_3$ with R = Er, Tm, Yb) have been measured in the 5.000–13.000 cm^{-1} infrared spectral range as a function of temperature between 8 and 300 K. A series of transitions has been assigned to the trivalent rare-earth ions in trigonal crystal field. Some of the Stark components of the rare-earth multiplets split below T_N interpreted as the Néel-temperature due to antiferromagnetic ordering. The Néel-temperatures obtained for the three compounds investigated decrease with increasing lattice constant (*a*).

Design and fabrication of diffractive optical elements and waveguides by ion implantation. — Slab and channel waveguides have been designed and fabricated in erbium doped tellurite glass samples via repeated implantation of N^+ ions using two out of the energies 3.5, 3.25, 3.0, 2.75 and 2.5 MeV at total implanted fluences of 4 x 10^{16} ions/cm^2 to suppress leaky modes detected in waveguides fabricated with single-energy implantation at 3.5 MeV. Spectroscopic ellipsometric measurements proved the existence of relatively broad implanted barrier layers (up to a thickness of 0.8 μm) in the waveguides. Thin films of silica of various thicknesses (50 nm to 150 nm) have been fabricated on silicon substrates by chemical vapour deposition (CVD) and subsequent implantation with N^+ or Ar^+ ions of energies of 20 and 50 keV, respectively.

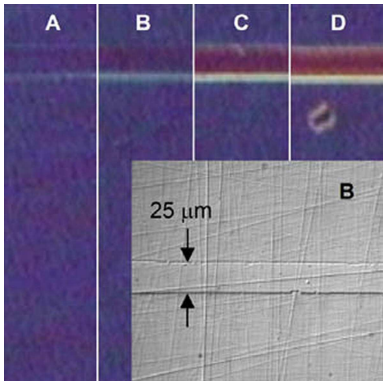

Fig.2. *Interference phase contrast microscopic images of the implanted channel waveguides in Er:Te glass. The applied fluences of 0.5, 1, 2 and 4 x 10^{16} N^+/cm^2 are denoted as A, B, C and D, respectively. Higher colour contrast indicates higher refractive index modulation. Conventional optical microscopic image of sample B is also shown in the inset for comparison.*

Optical phase diffraction gratings have been designed and fabricated in Pyrex glass samples via irradiation with focussed proton microbeams of 1 MeV energy and of 1 μm x 1 μm lateral size. Quasi-Gaussian refractive index profiles have been achieved due to lateral straggling of the protons in the target material.

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Grants and international cooperations

OTKA K 60086 Spectroscopic studies of photon-induced electron transport for data handling and medical applications (G. Corradi, 2006-2011)

OTKA K 68688 Fabrication of waveguides and diffractive optical elements via ion implantation (T. Lohner, Research Institute for Technical Physics and Materials Science HAS, contributors I. Bányász and A. Watterich, 2007 – 2012)

OTKA CK 80896 Scintillator materials for medical imaging purposes (L. Kovács, 2010-2013)

OTKA K 83390 Resonant optical processes in solids (L. Kovács, 2011-2015)

Hungarian – German project (P-MÖB/840 and DAAD PPP-Projekt 50445542, respectively) The effect of composition on the light-induced absorption of nonlinear-optical frequency converters of niobate and borate types (G. Corradi, 2010-2011)

HAS – CNR Application of ion implantation to the fabrication of integrated optical devices (I. Bányász, 2010-2012), Italian partner: MDF Laboratory, IFAC, Sesto Fiorentino

HAS – Estonian Academy of Sciences joint project: Radiation induced effects in pure and doped wide-gap borate crystals (G. Corradi, 2010-2012)

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Article in Hungarian

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See also Q.3., S.14.

S. QUANTUM OPTICS AND QUANTUM INFORMATICS

P. Ádám, J. Asbóth, Z. Darázs[#], A. Dombi[#], P. Domokos, A. Gábris, J. Janszky, O. Kálmán, L. Kecskés[#], Zs. Kis, T. Kiss, B. Kollár[#], Z. Kurucz, D. Nagy, V. Szalay, G. Szirmai, G. Tóth, A. Vukics

Cavity QED, Bose-Einstein condensates, many-body physics. — We developed a mean-field model describing the Hamiltonian interaction of ultracold atoms and the optical field in a cavity. The Bose-Einstein condensate is properly defined by means of a grand-canonical approach, and the relevant excitation modes are taken into account beyond the two-mode subspace. The self-organization, which is equivalent to the Dicke-type quantum phase transition in the two-mode subspace, has been described in this extended space. All the second-order correlations of the coupled atom field and radiation field hybrid bosonic system have been calculated, including the entanglement between the two types of fields.

The quantum phase transition of the Dicke model has been observed recently in this system formed by motional excitations of a laser-driven Bose-Einstein condensate coupled to an optical cavity. However, the cavity-based system is intrinsically open: photons leak out of the cavity where they are detected. Even at zero temperature, the continuous weak measurement of the photon number leads to an irreversible dynamics toward a steady state. In the framework of a generalized Bogoliubov theory, we show that the steady state exhibits a non-equilibrium quantum phase transition. We find that the critical point and the mean field are only slightly modified with respect to the phase transition in the ground state. However, the critical exponents of the singular quantum correlations are significantly different in the two cases. There is also a drastic modification of the atom-field entanglement, since the divergence of the logarithmic negativity of the ground state at the critical point is suppressed and a finite entanglement is found in the steady state.

We studied the excitation dynamics of a spin ensemble coupled to a single cavity mode in the Jaynes-Cummings regime with emphasis on ensemble's inhomogeneous broadening. We showed that the width and shape of the inhomogeneity have striking influence on the dynamics of the cavity-ensemble system and may lead to narrowing of the linewidth of the collective states. We underpinned our findings with the examples of a Gaussian and a Lorentzian profile of the inhomogeneity.

Quantum information processing, quantum walks, chaotic dynamics of entangled qubits. — The phenomenon that sensitivity to initial conditions leads to chaotic dynamics in classical physics is well-known. Similar phenomena in closed quantum systems are, however, excluded by the quantum unitary evolution. In the case of open quantum systems the restriction to unitarity is lifted. Entanglement purification, i.e., selection of certain systems from an ensemble of identical systems based on the results of partial measurements, can be regarded as a generalized feedback mechanism. The nonlinear dynamics resulting from such generalized feedback has recently been shown by us to lead in certain cases to true chaos.

We investigated the dynamics of an ensemble of identically prepared two-qubit systems which is subjected to the iteratively applied measurements and conditional selection of a typical entanglement purification protocol. The resulting dynamics exhibits strong sensitivity to initial conditions. For one class of initial states two types of islands characterize the asymptotic limit. They correspond to a separable and a fully entangled

[#] PhD student

two-qubit state, respectively, and their boundaries form fractal-like structures. Our results demonstrate that the typical dynamical procedure applied in entanglement purification protocols may lead to truly chaotic evolution of entanglement.

Molecular dynamics. — A first principles quantum mechanical calculation of the vibrational energy levels and transition frequencies associated with protons in stoichiometric $LiNbO_3$ single crystal has been carried out. The theoretically calculated transition frequencies agree within 1% with those experimentally determined, and they have allowed the assignment of one of the hitherto unassigned bands as a combination of the stretching and the bending of lower fundamental frequency.

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Grants and international cooperations

Momentum Program, Quantum Measurement Theory in Hybrid Mesoscopic Couplers and Networks (P. Domokos 2011-2015)

NKTH ERC_HU_09 OPTOMECH: Optomechanical coupling: extending Cavity Quantum Electrodynamics (P. Domokos 2010-2014)

OTKA K83858: Quantum optical and quantum information processing networks and their nonclassical properties (T. Kiss, 2011-2015)

FP7 Initial Training Network, CCQED Circuit and Cavity Quantum Electro-Dynamics (P. Domokos 2011-2014)

TéT, Hungarian-Czech Bilateral Intergovernmental S&T Cooperation (CZ-11/2009): Quantifying non-classicality in quantum walks and quantum optical networks (T. Kiss, 2010-2012)

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S.14. Szalay V, Lengyel K, Kovacs L, Timon* V, Hernandez-Laguna* A; Vibrations of H+(D+) in stoichiometric $LiNbO_3$ single crystal; J Chem Phys; **135**, 124501/1-19 2011

S.15. Wesenberg* J H, Kurucz Z, Mølmer* K; Dynamics of the collective modes of an inhomogeneous spin ensemble in a cavity; *Phys Rev A;* **83**, 023826/1-7, 2011

S.16. Xuereb* A, Domokos P, Horak* P, Freegarde* T; Cavity cooling of atoms: within and without a cavity; *Eur Phys J D*; **65**, 273, 2011

S.17. Zamora* A, Szirmai G, Lewenstein* M; Layered quantum Hall insulators with ultracold atoms; *Phys Rev A*; 84, 053620/1-6, 2011

S.18. Kálmán O, Kiss T, Fortágh* J, Domokos P; Quantum galvanometer by interfacing a vibrating nanowire and cold atoms; *NanoLetters*, accepted for publication

S.19. Koniorczyk* M, Szabó* L, Ádám P; Hardy's paradox and entangled structure of forward scatteres waves, *Phys Rev A*; accepted for publication

S.20. Szalay V, Szidarovszky* T, Czakó* G, Császár* AG; A paradox of grid-based representation techniques: accurate eigenvalues from inaccurate matrix elements; *J Math Chem;* accepted for publication

S.21. Vitagliano* G, Hyllus* P, Egusquiza* IL, Tóth G; Optimal spin squeezing inequalities for arbitrary spin; *Phys Rev Lett*; accepted for publication

Conference proceeding

S.22. Domokos P, Xuereb* A, Horak* P, Freegarde* T; Efficient optomechanical cooling in one-dimensional interferometers; *Laser Refrigeration of Solids IV;* edited by R. Epstein an M. Sheik-Bahae Proc. of SPIE; **7951**, 79510B; 1-11, 2011; doi: 10.1117/12.880045

See also: R.2., R.4.

T. SEMICONDUCTOR NANOSTRUCTURES

Á. Gali, D. Beke[#], T. Demjén[#], T. Hornos, V. Ivády[#], H. Pinto, K. Szász[#], M. Vörös[#], V. Zólyomi

The research team is active in three different main fields: to develop new type of i) biomarkers, ii) ultrasensitive magnetometers, and iii) 3rd generation solar cells.

Biomarkers. — Particularly, silicon carbide (SiC) nanocrystals were studied by theory and experiments in the research field of biomarkers. The experimental group developed a new method to fabricate SiC nanoparticles that were studied by infrared spectroscopy sensitive to the surface vibration modes. C=O local vibration modes as well as Si-O related vibration modes were found but no Si-H bonds. Previous results obtained in our *ab initio* calculations are in line with these findings.

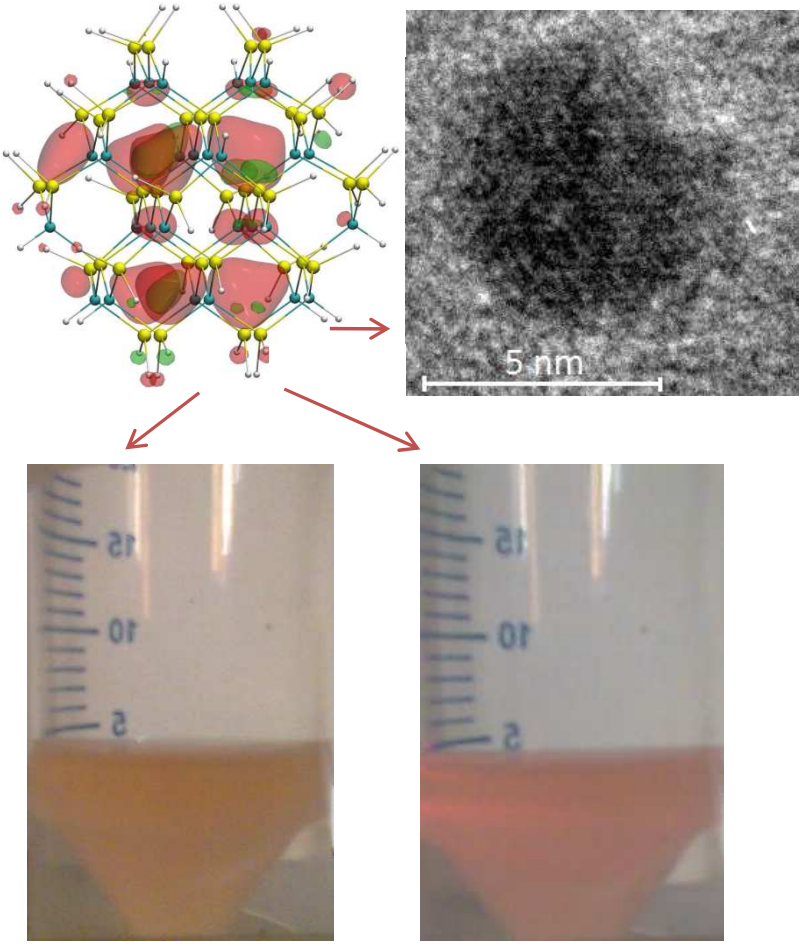

Fig. 1. *Upper left corner: Model of hydrogen terminated silicon carbide (SiC) nanocrystal (NC) where smaller(larger) balls represent carbon(silicon) atoms. The lobes show the charge density of the highest occupied molecular orbital. Upper right corner: high resolution transmission electron microscope image of our fabricated SiC NC. SiC colloid samples with and without molybdenum dopant as indicated below the figures.*

According to our idea, it would be desirable to introduce color centers in SiC nanoparticles in order to have more efficient fluorescence. Our calculations have shown that tungsten, molybdenum and other metal impurities may provide emission in the infrared region. These results have been presented in a keynote talk at the latest conference of International Conference on Silicon Carbide and Related Materials. The experimental group is working on the realization of these ideas as shown in Figure 1.

[#] PhD student

Ultrasensitive magnetometer. — Realization of ultrasensitive magnetometer is based on the peculiar properties of nitrogen-vacancy defect in diamond. The local vibration modes of this defect were calculated and analysed. In addition, a very detailed group theory analysis on its fine electronic structure was given in collaboration with Harvard University. Besides the hyperfine tensors were determined in detail and compared to new experimental data. In collaboration with the 3rd Physics Institute and Research Center SCoPE, University of Stuttgart, we could show that the negatively charged nitrogen-vacancy defect is temporarily ionized during the excitation process. Other important carbon based systems have been also studied. Carbon nanotubes and graphene are nanoscale materials with high potential for use in applications, especially in nanoelectronics. We have performed theoretical studies on various aspects of these materials. These include a first principles level study of electron-phonon coupling in graphene to help understand the behaviour of non-zone-center LO-LA phonons, a first principles study of the density of states in carbon nanotubes in relation to their weak ESR signal, and a study of carbon hyperfine coupling in carbon nanotubes. The resonance Raman spectroscopy of graphite and graphene was also reviewed.

3rd generation solar cells. — We studied the effect of shape on the absorption properties of small semiconductor nanocrystals that may be applied in nanocrystal based solar cells. We found that the absorption is enhanced in the appropriate energy region when the symmetry is reduced. In addition, we could achieve a breakthrough in first principles calculation of impact ionization rates in these nanocrystals. We applied the time-dependent density functional theory to calculate the excitation of point defects in semiconductors.

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Grants and international cooperations

EU FP7 No. 270197: DIAMANT-Diamond based atomic nanotechnologies (Á. Gali, 2011-2014)

PRACE Distributed European Computing Initiative (DECI-7) project DIAVIB, (Á. Gali, 2011-2012)

Publications

Articles

T.1. Ivády V, Gällström* A, Son* NT, Janzén* E, Gali Á; Asymmetric split-vacancy defects in SiC polytypes: a combined theoretical and electron spin resonance study; *Physical Review Letters*; **107,** 195501, 2011

T.2. Gali Á, Kaxiras* E, Zimanyi* GT, Meng* S; Effect of symmetry breaking on the optical absorption of semiconductor nanoparticles; *Physical Review B*; **84**, 035325, 2011

T.3. Son* NT, Gali Á, Szabó* Á, Bickermann* M, Ohshima* T, Isoya* J, Janzén* E; Defects at nitrogen site in electron-irradiated AlN; *Applied Physics Letters*; **98**; 242116, 2011

T.4. Gali Á; Time-dependent density functional study on the excitation spectrum of point defects in semiconductors; *physica status solidi b*; **248,** 1337-1346, 2011

T.5. Deák* P, Gali Á, Aradi* B, Frauenheim* T; Accurate gap levels and their role in the reliability of other calculated defect properties; *physica status solidi b*; **248**, 790-798, 2011

T.6. Waldherr* G, Beck* J, Steiner* M, Neumann* P, Gali Á, Frauenheim* Th, Jelezko* F, Wrachtrup* J; Dark states of single nitrogen-vacancy centers in diamond unraveled by single shot NMR; *Physical Review Letters*; **106**, 157601, 2011

T.7. Maze* JR, Gali Á, Togan* E, Chu* Y, Trifonov* A, Kaxiras* E, Lukin* MD; Properties of nitrogen-vacancy centers in diamond: the group theoretic approach; *New Journal of Physics*; **13**, 025025, 2011

T.8. Gali Á, Simon* T, Lowther* JE; An ab initio study of local vibration modes of the nitrogen-vacancy center in diamond; *New Journal of Physics*; **13**, 025016, 2011

T.9. Smeltzer* B, Childress* L, Gali Á; ^{13}C hyperfine interactions in the nitrogen-vacancy centre in diamond; *New Journal of Physics*; **13**, 025021, 2011

T.10. Heiss* M, Conesa-Boj* S, Ren* J, Tseng* H-H, Gali Á, Rudolph* A, Uccelli* E, Peiró* F, Ramon Morante* J, Schuh* D, Reiger* E, Kaxiras* E, Arbiol* J, Fontcuberta i Morral* A; Direct correlation of crystal structure and optical properties in wurtzite/zinc-blende GaAs nanowire heterostructures; *Physical Review B*; **83,** 045303, 2011

T.11. Carlsson* P, Son* NT, Gali Á, Isoya* J, Morishita* N, Ohshima* T, Magnusson* B, Janzén* E; EPR and ab initio calculation study on the EI4 center in 4H- and 6H-SiC; *Physical Review B*; **82,** 235203, 2010

T.12. Ferone R*, Wallbank JR*, Zólyomi V, McCann E*, Fal'ko VI*; Manifestation of LO-LA phonons in Raman scattering in graphene; *Sol Stat Commun*; **151,** 1071-1074, 2011

T.13. Zólyomi V, Koltai J*, Kürti J*; Resonance Raman spectroscopy of graphite and graphene; *physica status solidi (b)*; **248,** 2435-2444, 2011

T.14. Szirmai P*, Fábián G*, Dóra B*, Koltai J*, Zólyomi V, Kürti J*, Nemes NM*, Forró L* Simon F*; Density of states deduced from ESR measurements on low-dimensional nanostructures; benchmarks to identify the ESR signals of graphene and SWCNTs; *physica status solidi (b)*; **248,** 2688-2691, 2011

T.15. Beke D, Szekrényes Zs, Balogh I, Veres M, Fazakas É, Varga LK, Kamarás K, Czigány* Zs, Á Gali; Characterization of luminescent silicon carbide nanocrystals prepared by reactive bonding and subsequent wet chemical etching; *Applied Physics Letters*; **99**, 213108/1-3, 2011

Conference proceedings

T.16. Vörös* M, Demjén T, Gali Á; The absorption of diamondoids from time-dependent density functional calculations; *MRS Proceedings*; **1370,** mrss11-1370-yy02-07, 2011

T.17. Vörös* M, Deák* P, Frauenheim* Th, Gali Á; Influence of oxygen on the absorption of silicon carbide nanoparticles; *Mater. Sci. Forum*; **679-680,** 520-523, 2011

T.18. Vörös* M, Deák* P, Frauenheim* Th, Gali Á; Time-dependent density functional calculations on hydrogenated silicon carbide nanocrystals; *Mater. Sci. Forum;* **679-680,** 516-519, 2011

T.19. Hornos T, Gali Á, Svensson* BG; Large-scale electronic structure calculations of vacancies in 4H-SiC using the Heyd-Scuseria-Ernzerhof screened hybrid density functional; *Mater Sci Forum*; **679-680,** 261-264, 2011

T.20. Gali Á; Defects in SiC: theory; *Mater. Sci. Forum*; **679-680,** 225-232, 2011

See also: A.7.

EDUCATION

Graduate and postgraduate courses, 2011

— Solid-state physics (J. Sólyom, ELTE[2])

— Stochastic processes (R. Juhász, PPKE[3])

— Completely integrable many-body systems (F. Woynarovich, ELTE)

— Statistical physics (F. Iglói , SZTE[4])

— Application of statistical physics (F. Iglói, SZTE)

— Disordered systems (F. Iglói, SZTE)

— Many body problem II. (P. Szépfalusy, ELTE)

— Electrons in solids (I. Tüttő, ELTE)

— Nanomagnetism (J. Balogh, ELTE)

— Solid state research II. (I. Vincze, ELTE)

— Infrared and Raman spectroscopy (K. Kamarás, BME)

— Macromolecules I. (S. Pekker ELTE)

— Phase field modelling and solidification (L. Gránásy, T. Pusztai, G. I. Tóth, and G. Tegze, Rolls-Royce University Technology Centre, Cambridge University, UK)

— Physics of liquid crystals and polymers (Á. Buka and N. Éber, ELTE)

— Liquid crystals, their chemistry and chemical physics (K. Fodor-Csorba, ELTE)

— Pattern formation in complex systems (Á. Buka and T. Börzsönyi, ELTE)

— Group theory in solid state research (G. Kriza, BME)

— Superconductivity (G. Kriza, BME)

— Nanophase metals (I. Bakonyi, ELTE)

— Electrodeposition of metals (L. Péter, ELTE)

— Mathematical analysis – theory and practice (B. Tóth, ZMNE[5])

— Control theory (J. Füzi, PTE[6])

— Electronics (J. Füzi, PTE-PMMK)

— Digital Control (J. Füzi, PTE-PMMK)

— Machine elements I. (L. Zoltan SZIE[7])

— Machine elements II. (L. Zoltan SZIE)

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[2] ELTE = Loránd Eötvös University, Budapest

[3] PPKE = Pázmány Péter Catholic University

[4] SZTE = University of Szeged

[5] ZMNE = Zrínyi Miklós National Defense University, Budapest

[6] PTE = University of Pécs

[7] SZIE = Szent István University

— Computer Aided Engineering (L. Zoltan SZIE)

— Disorder in condensed phases (L. Pusztai, ELTE)

— Physics of amorphous matter I.-II. (M. Koós, SZTE)

— Raman spectroscopy, part of the course Experimental methods in materials science (M. Veres, BME)

— Infrared vibrational spectroscopy, part of the course Experimental methods in materials science (L. Kovács, BME)

— Quantum mechanics I-II (J. Janszky, PTE)

— Numerical methods (P. Ádám, PTE)

— Quantum mechanics II. (P. Ádám, PTE)

— Theoretical physics III. (P. Ádám, PTE)

— Open quantum systems (P. Ádám, PTE)

— Probability theory (P. Ádám, PTE)

— Cavity quantum electrodynamics (P. Domokos, BME, ELTE)

— Measurement in quantum mechanics and quantum optics (T. Kiss, PTE)

— Calculus (B. Kollár, PTE)

— Mathematical methods in physics III. (B. Kollár, PTE)

— Introduction to quantum optics (Z. Kis, ELTE)

— Coherent control of quantum systems (Z. Kis, BME)

Laboratory practice and seminars

— Solid-state physics seminar (I. Tüttő, ELTE)

— Stochastic processes (R. Juhász, PPKE)

— Laboratory for solid state physics, Preparation and crystallization of metallic glasses (I. Vincze, ELTE)

— Laboratory practice (T. Pusztai, ELTE)

— Infrared and Raman spectroscopy (K. Kamarás, BME)

— Experiments on liquid crystals (Á. Buka, N. Éber, and T. Tóth-Katona, ELTE)

— Physical chemistry laboratory practice (L. Péter and B. Tóth, ELTE)

— Laboratory practice in solid state physics and materials science (K. Tompa and M. Bokor, ELTE)

— Control theory practice (J. Füzi, PTE)

— Electronics laboratory practice (J. Füzi, PTEÖ

— Practice course in experimental physics for engineer-physicists (A. Szakál, BME)

— Practice course in electrodynamics for energy-engineers (A. Szakál, BME)

— Laboratory practice in neutron diffraction (L. Pusztai, ELTE)

— Raman spectroscopy, part of the course Experimental methods in materials science (M. Veres, BME)

— Infrared vibrational spectroscopy, part of the course Experimental methods in materials science (L. Kovács, BME)

— Quantum optics seminar (Z. Kis, BME)

Diploma works

D. Varjas (BME): Effects of magnetic anisotropy in classical Heisenberg pyrochlore antiferromagnets (MSc, 2011) (Supervisor: K. Penc)

G. Homa (ELTE): Properties of superfluid quantum gases on Fermi gas resonance (Supervisors: P. Szépfalusy and A. Csordás*).

G. Törös (BME, MSC): Shear induced alignment of elongated particles (Supervisor: T. Börzsönyi)

L. Zoltán (SZIE) Design of a sample holder for a Small Angle Neutron Scattering Instrument (Supervisors: J. Nagy, J. Füzi)

L. Rátkai (ELTE): Short range ordering in covalent amorphous alloys (MSc, Supervisor: P. Jóvári)

B. Bódi (BME): Optical control of an ultrafast electron source, (Supervisor: P. Dombi)

D. Csáti (SZTE): Development of a modelocked Yb-fiber oscillator/amplifier system, for nonlinear microscopy (Supervisor: R. Szipőcs)

É. Tichy-Rács (ELTE): Preparation and study of nano-particles of alkali-orthoborate scintillator materials (Supervisor: K. Polgár, consultant: Katalin Perényi, ELTE)

G. Kónya (ELTE, MSc): Bose-Einstein condensates in optical resonators (Supervisor: P. Domokos)

P. Sinkovicz (ELTE, MSc): Theoretical study of chiral spin liquid states in an ultracold gas of fermionic atoms (supervisor: G. Szirmai)

L. Ábrok (ELTE, Physicist BSc): Propagation of the de Brogile waves of molecules (supervisor: Z. Kis)

T. Szarvas (BME, Physicist MSc) : Modeling the propagation of electromagnetic waves in 2D photonic crystals (supervisor: Z. Kis)

Ph. D. students

G. Barcza (ELTE): Development and application of the non-local density matrix renormalization group (non-local DMRG) method to low-dimensional spin and fermionic models (Supervisors: Ö. Legeza and F. Gebhard*)

I. Hagymási (ELTE): Heavy-fermion behaviour in the periodic Anderson model (Supervisor: J. Sólyom)

M. Lajkó (BME): Theoretical studies of strongly frustrated spin and charge systems (Supevisor: K. Penc)

J. Romhányi (BME): Bond and plaquette ordering in interacting electron systems (Supervisor: K. Penc)

I. Kovács (ELTE): Renormalization of disordered quantum systems (Supervisor: F. Iglói)

E. Simon (ELTE): Numerical investigation of interactions between magnetic impurities (Supervisor: B. Újfalussy)

K. Németh (ELTE): Chemical functionalization of carbon nanotubes (Supervisor: K. Kamarás)

B. Botka (BME): Raman spectroscopy of carbon nanotube peapods (Supervisor: K. Kamarás)

Á. Pekker (BME): Far-infrared spectroscopy of carbon nanotubes (Supervisor: K. Kamarás)

Zs. Szekrényes (BME): Infrared spectroscopy of self-assembled structures on surfaces (Supervisor: K. Kamarás)

H. M. Tóháti (SZTE): Optical spectroscopy of confined luminescent materials (Supervisor: K. Kamarás)

Gy. Tegze (ELTE): Phase field modeling of microstructures (Supervisor: L. Gránásy)

Gy. Tóth (BME): Engineered self-organised multi-component structures with novel controllable electromagnetic functionalities (Supervisor: L. Gránásy)

C. Nitin: Optical spectroscopy of confined luminescent materials (Advisor: Rudolf Gross, Walther-Meissner-Institut, Garching, Germany, Hungarian Supervisor: K. Kamarás)

D. Kocsis (ELTE): Spectroscopy on filled carbon nanotube systems (Supervisor: K. Kamarás

P. Salamon (ELTE): Flexoelectricity in liquid crystals (Supervisor: N. Éber)

B. Szabó (ELTE): Experimental investigations of granular flows (Supervisor: T. Börzsönyi)

K. Neuróhr (ELTE): Electrochemical preparation of multilayers with giant magneto-resistance (Supervisor: L. Péter)

B. Tóth (ELTE): Giant magnetoresistance (GMR) in multilayers (Supervisors: I. Bakonyi and L. Péter)

K. Szász (ELTE): Study of the magnetic and transport properties of nanowires (Supervisors: I. Bakonyi and L. Péter)

T. Verebélyi (ELTE): NMR and DSC study of protein solutions (Supervisor: K. Tompa)

Z. László (SZIE): Magnetic bearings for neutron beam phase space tailoring (Supervisors: J. Nagy, J. Füzi)

M. Markó (BME): Atomic resolution neutron holography (Supervisor: L. Cser)

J. Orbán (BME): Investigation and development of signal processing electronics for position sensitive particle counters (Supervisor: L. Rosta and Cs. Süközd*)

A. Szakál (BME); Investigation of the structure and dynamics of metal-hydrogen systems with neutron scattering (Supervisor: L. Cser)

R. Ünnep (ELTE); Study of self-assembly functional nano participles by neutron scattering (Supervisor: F. Mezei)

P. Rácz (BME): Development of femtosecond light and electron sources for high resolution methods (Supervisor: P. Dombi)

A. Kerekes (BME): Development of optical instrumentation for environmental measurements (Supervisor: A. Czitrovszky)

L. Himics (SZTE): Nanocrystalline diamonds for advanced applications (Supervisor: M. Koós)

P. Antal (ELTE): Generation and compression of femtosecond laser pulses in optical fibers and their application in non-linear optics (Suprevisor: R. Szipőcs)

K. György (ELTE): Study on solid sampling spectrochemical methods for characterization of the impurity ions and dopants of optical crystals. (Supervisor: L. Bencs)

É. Tichy-Rács (ELTE): Synthesis, crystallization and spectroscopy of rare-earth-alkaline ortho-borates (Supervisor: K. Polgár)

I. Hajdara (PTE): Spectroscopy of ferroelectric oxide crystals (Supervisor: L. Kovács)

Z. Darázs (ELTE): Quantum controll with measurements (Supervisior: T. Kiss and A. Csordás*)

A. Dombi (ELTE): Quantum dynamics of atomic motion in multimode optical resonator fields (supervisor: P. Domokos)

L. Kecskés (PTE): Complex chaos in the dynamics of qubits (Supervisor: T. Kiss)

B. Kollár (PTE): Quantum information in quantum-optical networks (Supervisor: T. Kiss)

D. Nagy (BME): Collective effects in the laser cooling of neutral atoms (Supervisor: P. Domokos)

Á. Varga (PTE): Quantum state discrimination (Supervisor: P. Ádám)

Dissertations

Á. Gali (D.Sc): Density functional study on the electronic structure of point-defects in silicon carbide, silicon carbide nanotubes, and diamonds.

T.A. Tóth (PhD, EPFL): Quadrupolar ordering in two-dimensional S=1 systems (Supervisors: F. Mila and K. Penc)

Á. Pekker (PhD, BME): Wide range optical studies on single walled carbon nanotubes, Budapest University of Technology and Economics (Supervisor: K. Kamarás)

É. Fazakas (PhD, ELTE): Novel amorphous and nanostructured Al-based alloys (Supervisors: I. Bakonyi and L.K. Varga)

A. Meiszterics (PhD, ELTE); Calcium containing bioceramics prepared by sol-gel method and their structure investigation (Supervisor: L. Rosta and K. Sinkó*)

G. Nagy (PhD, ELTE, Université de Grenoble): Structure and dynamics of photosynthetic membranes as revealed by neutron scattering (Supervisors: L. Rosta, J. Peters*, P. Timmins*, Gy. Garab)

V. Mile (PhD, ELTE): Structural studies of aqueous cesium-halide solutions (Supervisor: L. Pusztai)

AWARDS

— J. Janszky: Commander Cross of the Order of Merit of the Hungarian Republic (Civilian)

— P. Szépfalusy: Hungarian Order of Merit Cross with the Star

— J. Sólyom: Széchenyi Prize

— N. Kroó: Prima Primissima Prize

— L. Vitos: Lee Hsun Lecture Award, Chinese Academy of Sciences (2011)

— L. Vitos: Vision Award 2010, Ångström Materials Academy (ÅMA).

— Z. Donkó: Award of the Section of Physical Sciences of the Hungarian Academy of Sciences, 2011

— R. Szipőcs, Patent Excellence Award of the Hungarian Academy of Sciences (2011)

— P. Domokos: Momentum Prize of the Hungarian Academy Sciences

— J. Asbóth: Junior Príma Prize

— L. Péter: SZFKI Annual Publication Award (2011)

— P. Hartmann: SZFKI Annual Publication Award (2011)

— P. Dombi, P. Rácz: SZFKI Applied Research Award (2011)

— I. Hagymási: Pro Scientia gold medal of the Scientific Students' Association Council

— I. Hagymási: Best poster award on the Physics of Magnetism 2011 Conference

— G. Bortel: Bolyai Grant (2011-2014)

— P. Jóvári: Bolyai Grant (2008-2011)

— P. Dombi: Bolyai Grant (2011-2014)

— P. Hartmann: Bolyai Grant (2008-2011)

— K. Kutasi: Bolyai Grant (2008-2011)

MEMBERSHIPS

J. Sólyom:	— Chairman of the Physics Section of the Hungarian Academy of Sciences
	— President of Physical Section of HAS
Á. Gali:	— Member of European Conference on Silicon Carbide and Related Materials Steering and Program Committee
	— Member of International Conference on Silicon Carbide and Related Materials Program Committee
K Penc:	— Member of the Steering committee for the ESF "Highly Frustrated Magnetism" network activity
J. Balogh:	— Member of the International Board on the Application of the

Mössbauer effect, IBAME (2007-2012)

K. Kamarás:
— Editorial Board Member of the European Physical Journal B

G. Faigel:
— XFEL In-kind Review Committee member
— XFEL SAC member
— President of Physical Section of HAS

L. Gránásy:
— Member of the ESA Topical Team "Solidification of Containerless Undercooled Melts", SOL – EML
— Member of International Scientific Committee of the 3rd International Conference on Advances in Solidification Processes, (Aachen/Rolduc 2011)

Á. Buka:
— Member of the Editorial Board, Electronic-Liquid Crystal Communications
— Member of the International Advisory Board, International Liquid Crystal Conference
— Member of the National Scientific Research Fund OTKA, Physics Panel
— Member of the Solid State Physics Committee of HAS
— Member of the ERC Starting Grant, Condensed Matter Panel

K. Fodor-Csorba:
— Member of the ESF COST D35 Management Committee
— Board member of the Open Organic Chemistry Journal

N. Éber:
— Member of the International Liquid Crystal Society, Board of Directors
— Member of the Open Crystallography Journal, Editorial Board

I. Jánossy:
— Member of the Electronic-Liquid Crystal Communications, Editorial Board

I. Bakonyi:
— Elected Member of the General Assembly of HAS (2010-2012)
— I. Bakonyi, Member of the Solid State Physics Committee of HAS (2011-2014)
— Member of the Editorial Advisory Board (2005-), Journal of Materials Science and Technology (Bulgaria, Sofia)
— Member of the European Board (2006-), European Academy of Surface Technology (EAST)
— Member of the International Advisory Board, 1st Surface Technology Symposium (Istanbul, Turkey, 2011)
— Member of the EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)

L.K. Varga:
— Member of the International Organising Committee (2005-), International Conference on Soft Magnetic Materials (SMM)

	— Member of Advisory Committee (2004-), Czech and Slovak Conference on Magnetism (CSMAG)
L. Péter:	— Secretary of the EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)
	— Secretary of the Electrochemical Committee of HAS (2005-)
	— Representative for Hungary, International Society of Electrochemistry (2011-2013)
	— Council Member of Graduate School of Chemistry, ELTE (2009-)
	— Editor for Electrochemistry (Central European Journal of Chemistry, 2009-)
G. Kriza:	— Member of the Solid State Physics Committee of HAS (2007-2012)
	— Elected Member of the General Assembly of HAS (2007-2012)
	— Member of Ph.D. School of Physics, BME (2008-)
	— Member of Bolyai Fellowship Board, HAS (2010-)
	— Member of MTA Domus Hungarica Scientiarum et Artium Fellowship Board (2008)
K. Tompa:	— Member of the the Natural Science Committee of the Hungarian Scholarship Board (2011-2013)
	— Member of Ph.D. Council of ELTE (2008-2012)
L. Cser:	— International Scientific Advisory Council of BNC (Budapest Neutron Centre)
F. Mezei:	— International Scientific Advisory Council of BNC (Budapest Neutron Centre)
	— European Neutron Scattering Association (ENSA) Committee
	— Scientific Advisory Council of SNS (Spallation Neutron Source), Oak Ridge National Laboratory, USA
L. Rosta:	— International Scientific Advisory Council of BNC (Budapest Neutron Centre)
	— European Spallation Source, Steering Committee
N. Kroó:	— Vice-President of the Hungarian Academy of Sciences
	— Member of the Presidium of HAS
	— Chairman of the Research Infrastructure Committee of HAS
	— Chairman of the Committee of International Relations of HAS
	— Chair of the Governing Council of the Hungarian Research Infrastructure Program
	— Chair of the Rátz High School Prize

— Member of the Hungarian UNESCO Committee

— Chair of the Dennis Gabor International Prize Committee

— Member of the Scientific Council of the European Research Council

— Chairman of the Research Infrastructure Expert Group of ERA (EC)

— Member of the High Level Expert Group on Digital Libraries and Scientific Publications (EC)

— Member (former Chair) of the Section of Physical and Engineering Sciences of Academia Europaea

— Member of the Advisory Group on ESOF

— Member of the ELI_ALPS Scientific Advisory Committee

Z. Donkó:

— Conference series "Symposium of the Phenomena in Ionized Gases", Member of International Scientific Committee, 2006-

— Member of International Advisory Board of the Conference series "Strongly Coupled Coulomb Systems", 2007-

— Member of International Scientific Committee of the Conference series "Symposium on Application of Plasma Processes" 2008-

P. Hartmann:

— Conference series "Europhysics Conference on the Atomic and Molecular Physics of Ionized Gases" Member of International Scientific Committee, 2008-2014

K. Kutasi:

— Conference series “International Workshop on Nonequilibrium Processes in Plasma Physics and Studies of Environment, Member of International Scientific Committee, 2006-

A. Czitrovszky:

— Chairman of the Working Group Instrumentation in EAA

— Member of the Board of International Aerosol Association

— Member of Gesellschaft für Aerosolforschung

— President of the Hungarian Aerosol Society

— Member of the ELI_ALPS Scientific Advisory Committee

— Member of the Int. Organizing Committee of International Aerosol Conference (Manchester, 2011)

— Member of the Int. Program Committee of Int. Conf on Advanced Laser Technologies (Varna, Bulgaria, 2011)

— President of the Hungarian Branch of the European Optical Society

— Head of the Optical Chapter of the Scientific Society for Optics, Acoustics, Motion Pictures and Theatre Technology (Budapest)

— Member of the Editorial Board of “Fizikai Szemle”

— Chairman of the Optical Chapter of Loránd Eötvös Physical

	Society
	— Chairman of the Committee for the Lasers Physics and Spectroscopy in HAS
	— Member of the Int. Organizing Committee of International Aerosol Conference (Helsinki, 2010)
	— Member of the Int. Program Committee of Int. Conf on Advanced Laser Technologies (Egmont aan Zee, The Netherlands, 2010)
K. Polgár:	— Hungarian Advisor of the International Organization for Crystal Growth
	— International Advisory Board of the 4th European Conference on Crystal Growth ECCG-4
	— International Advisory Committee of the 17th Intern. Conference on Crystal Growth and Epitaxy (ICCGE-17)
L. Bencs:	— Editorial Board member of Environmental Monitoring and Management (Internat. Journal)
	— Editorial Board member of ISRN Analytical Chemistry
L. Kovács:	— Member of the International Advisory Committee, EURODIM-ICDIM
	— Member of the Hungarian National Committee, International Union of Crystallography
P. Domokos:	— Editor of the European Physical Journal D
	— Liaison Committee representative of the International Union of Pure and Applied Physics (IUPAP)
J. Janszky:	— Member of the Editorial Board of Nonlinear and Quantum Optics
	— Member of the Editorial Board of Problems in Physics
T. Kiss	— Member of the Commission on Quantum Electronics (C17) of the International Union of Pure and Applied Physics (IUPAP)

CONFERENCES

— **MAGFUM Swedish-Hungarian STINT workshop "Magneto-mechanical properties of complex functional materials"**, Danubius Hotel Sovata, Romania, 31 May - 4 June 2011, Main coordinator: L. Vitos

— **Joint Hungarian – American Workshop on Complex Fluids**, Sopron, Hungary, July 11 – 13, 2011. Organizer: I. Jánossy. Number of participants: 24. At the workshop researchers and students from Hungary, United States and other countries (Slovakia, Germany and Mexico) gave reports about their latest results in connection with complex fluids.

— The Neutron Spectroscopy Department in cooperation with MIRROTRON Co. organized a **Professional Training in Neutron Research and Instrumentation** workshop with the specific purpose of training in Residual Stress Neutron Diffraction for a group of scientists and engineers of the Institute of Nuclear Physics and Chemistry, Mianyang, China in the period of June 19 - July 16, 2011 (4 weeks). The training consisted of education in neutron scattering with specific orientation on neutron diffraction an strain scanning, including lectures given by leading scientists of the Budapest Neutron Centre (BNC) and renowned European experts invited by BNC as well as hands-on training using BNC neutron facilities.

— **CHARISMA – (Cultural Heritage Advanced Research Infrastructures: Synergy for a Multidisciplinary Approach to Conservation/Restoration)** is an EU-funded integrating activity project carried out in the FP7 Capacities Specific Programme "Research Infrastructures". It's 2nd Interim Meeting was held in Budapest at the Hungarian Academy of Sciences on March 3 to 4, 2011 with the participation of more than 60 experts from the the European Union partner institutes. The activity – including 21 European partner institutes – provides transnational access to most advanced scientific instrumentations and knowledge allowing scientists, conservators-restorers and curators to enhance their research at the field forefront.

— A symposium "**Concerted Actions in Research and Applications with Neutron Beams in Europe**" was organized by he International Atomic Energy Agency (IAEA) in collaboration with the Government of the Republic of Hungary through the Budapest Neutron Centre on 1-3 June 2011 in Budapest. The IAEA promotes networking, coalitions and regional collaboration to improve the efficient and sustainable utilization of Research Reactors (RRs). This workshop aimed to strengthen the cooperative efforts of the member institutions in the field of neutron beam research and applications. The meeting was attended by 39 participants from 14 Member States in Europe. The workshop covered several topics as research and industrial applications using various neutron beam techniques, recent modernization/upgrade projects related to neutron beam facilities, education and training using neutron beams.

— To mark the Hungarian Presidency of the European Union the annual Board meeting of the **Neutron Muon Integrated Infrastructure Initiative (NMI3)** project in FP7 was held on the 12th of May 2011 in Budapest, it was hosted by the Budapest Neutron Centre (BNC), and organised by the contribution of the Neutron Spectroscopy Department. This project gathers the 10 major European neutron source facilities and another 10 adjoining institutions to provide access and research opportunities for a wide community of researchers. Nearly 50 delegates of the project partners discussed the next 4 years plans

— The **European Neutron Scattering Association (ENSA)** held its first annual Committee meeting on the 13th of May 2011 in Budapest, it was hosted by the Budapest Neutron Centre, and organised by the Neutron Spectroscopy Department. This meeting was attended by 40 delegates and observers.

— **Light at Extreme Intensities**, Szeged, 14-18 November 2011, Member of local organizing comittee: Dombi P, 120 participants. The LEI conference provided the scientific communities involved in various sub-fields of ELI with an opportunity of meeting and discussing the most important scientific achivements, theoretical predictions and site construction matters towards the implementation of the research infrastructures at the ELI sites as well as the planning of the 200PW facility.

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