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2010

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

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Hungarian Academy of Sciences

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ANNUAL REPORT 2010

Edited by **V. Blázsik-Kozma, G. Konczos, B. Selmeci, I. Tüttő**

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Dear Reader,

It is my pleasure to hand over the 17th edition of the Annual Report of the Research Institute for Solid State Physics and Optics. Our institute has been operating in its present form following the reorganisation of the well-known Central Research Institute for Physics of the Hungarian Academy of Sciences in 1992. The mission of the institute is 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.

Our staff of 196 includes 130 scientists. This year we have published over 230 papers in highly ranked international journals and conference proceedings showing a steadily high publication activity over the last years. This year, two further volumes of the textbook: “Fundamentals of the Physics of Solids” by Jenő Sólyom were published.

An International Advisory Board was set up this year and began its work according to the Hungarian Academy of Sciences Act. During the first session principles of the future activity have been discussed and five current research topics have been thoroughly analysed by the Board.

In 2009, the President of the Hungarian Academy of Sciences launched its "Momentum - From Brain Drain to Brain Gain" program in order to support the reintegration of young, talented Hungarian researchers at home. One of the 2010-Year-winners, Ádám Gali will implement his research on the nanostructured materials in our Institute. In the framework of the National Technology Program, two new laboratories have been launched by Róbert Szipőcs: one for development of femtosecond fiber lasers and an other one for the application of nonlinear microscopy in pharmacological and diagnostic investigations. The program is financed by the National Office for the Technology Development (NKTH).

Several awards and nominations have acknowledged the achievements of our scientists. Katalin Kamarás and János Kollár have been elected as Corresponding Member of the Hungarian Academy of Sciences. Levente Vitos received the DSc title at the Hungarian Academy of Sciences. Nine of our young researchers have received their PhD degrees.

Kinga Kutasi won the national L’Oreal-UNESCO “For Women in Science” award in 2010 for her pioneering results in the study of plasma physics. Aladár Czitrovszky was awarded the International Gábor Dénes Prize for his work on laser applications. Géza Konczos received the Knight’s Cross Order of Merit of the Hungarian Republic for his achievements in materials research and science management. Last but not least Erika Eőry got the Diploma of Merit of the Secretary General HAS.

It has become a tradition of the institute to deliver prizes for outstanding publication activity and applied research, respectively. In 2010, the Publication Prize was awarded to

Péter Dombi for his papers concerning surface plasmons and femtosecond lasers. The Applied Research Prize was given to János Füzi for the development of novel neutron physical equipment and to Attila Tibor Nagy for the development and application of his dual wavelength optical particle spectrometer.

I hope this booklet will provide you with 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.

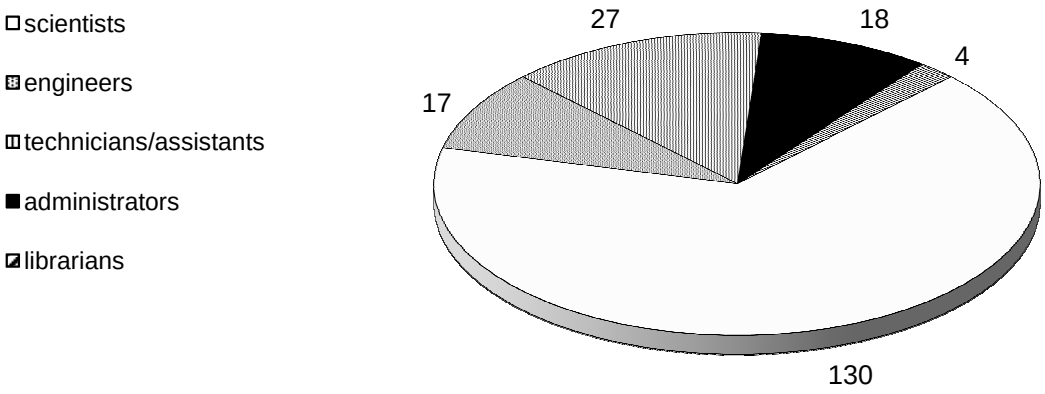
Budapest, December 4, 2010.

János Kollár
Director

KEY FIGURES

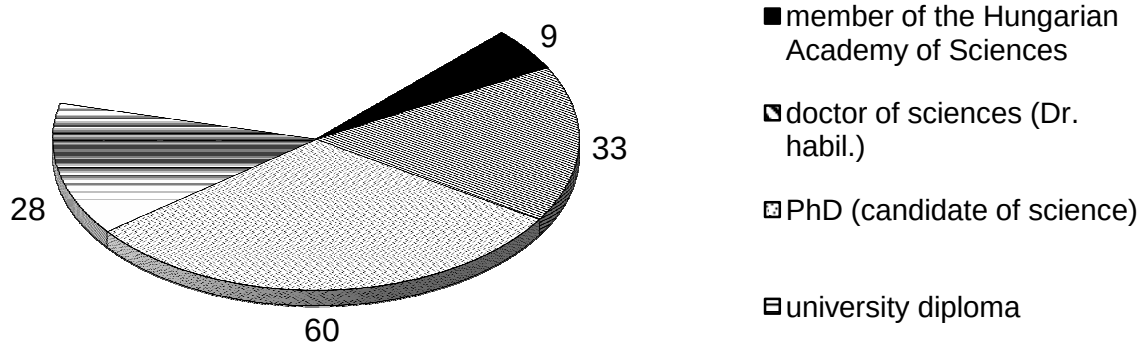
Permanent staff of the institute: 196 employees.

Its **distribution by professions**:

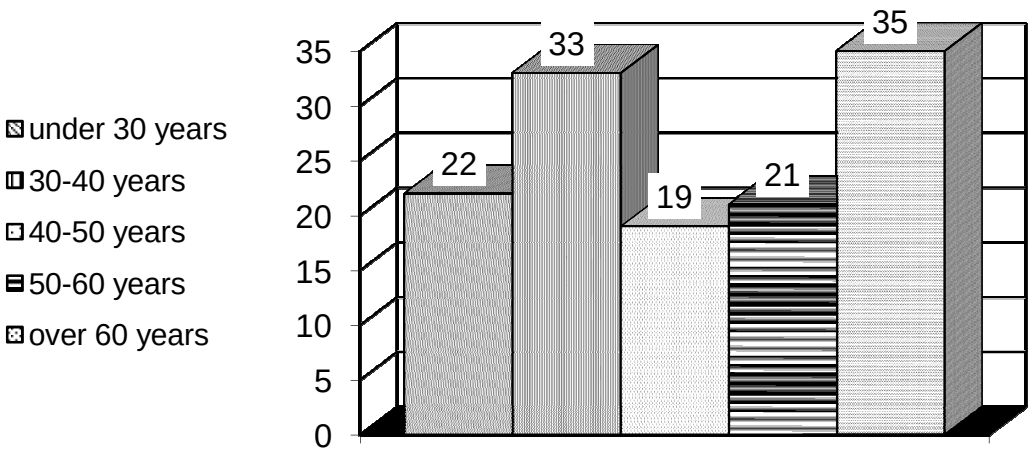


Distribution of scientists:

a) by scientific titles/degrees:

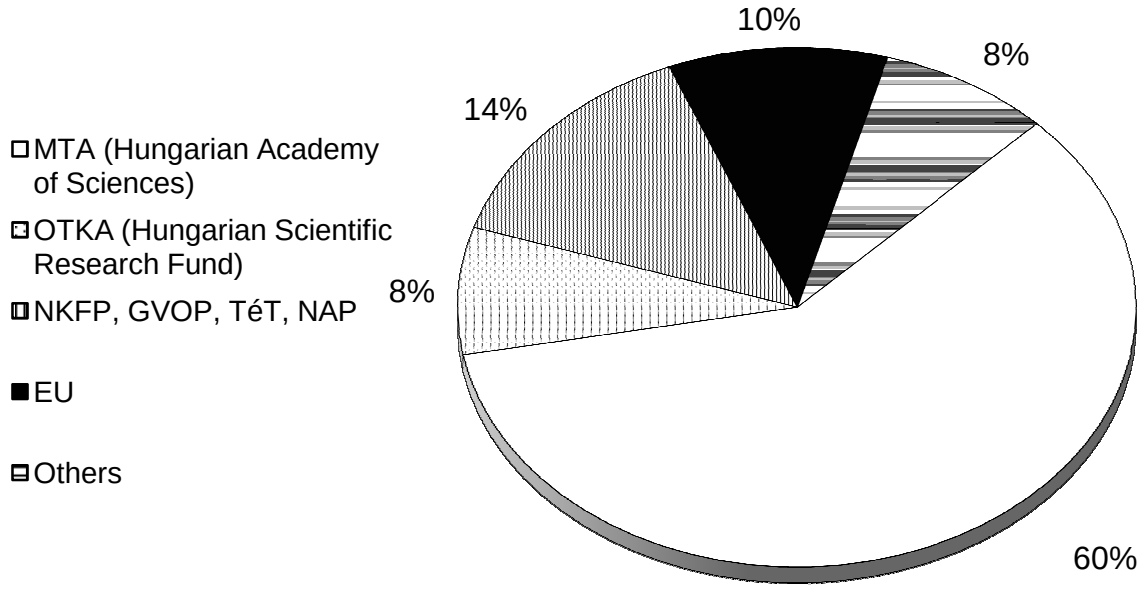


b) by age groups:

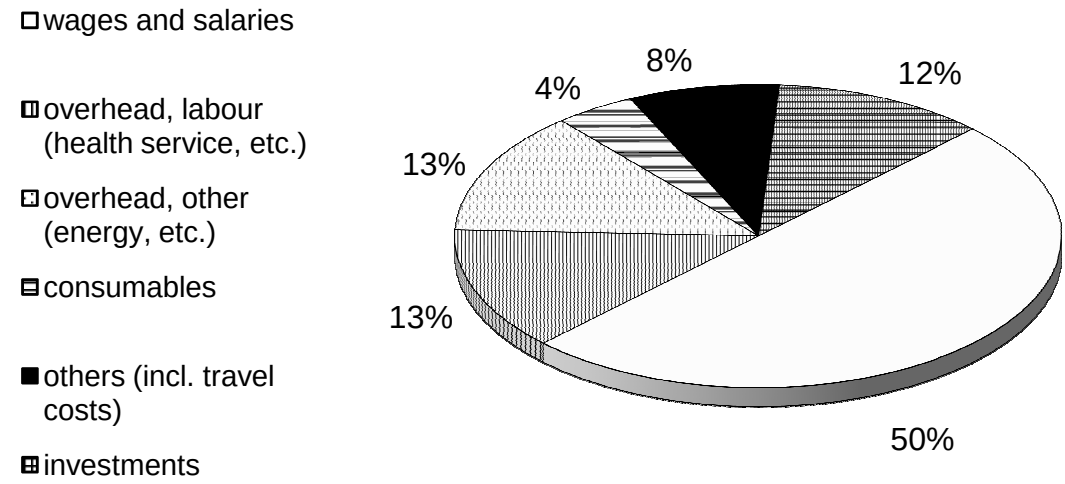


Financial management

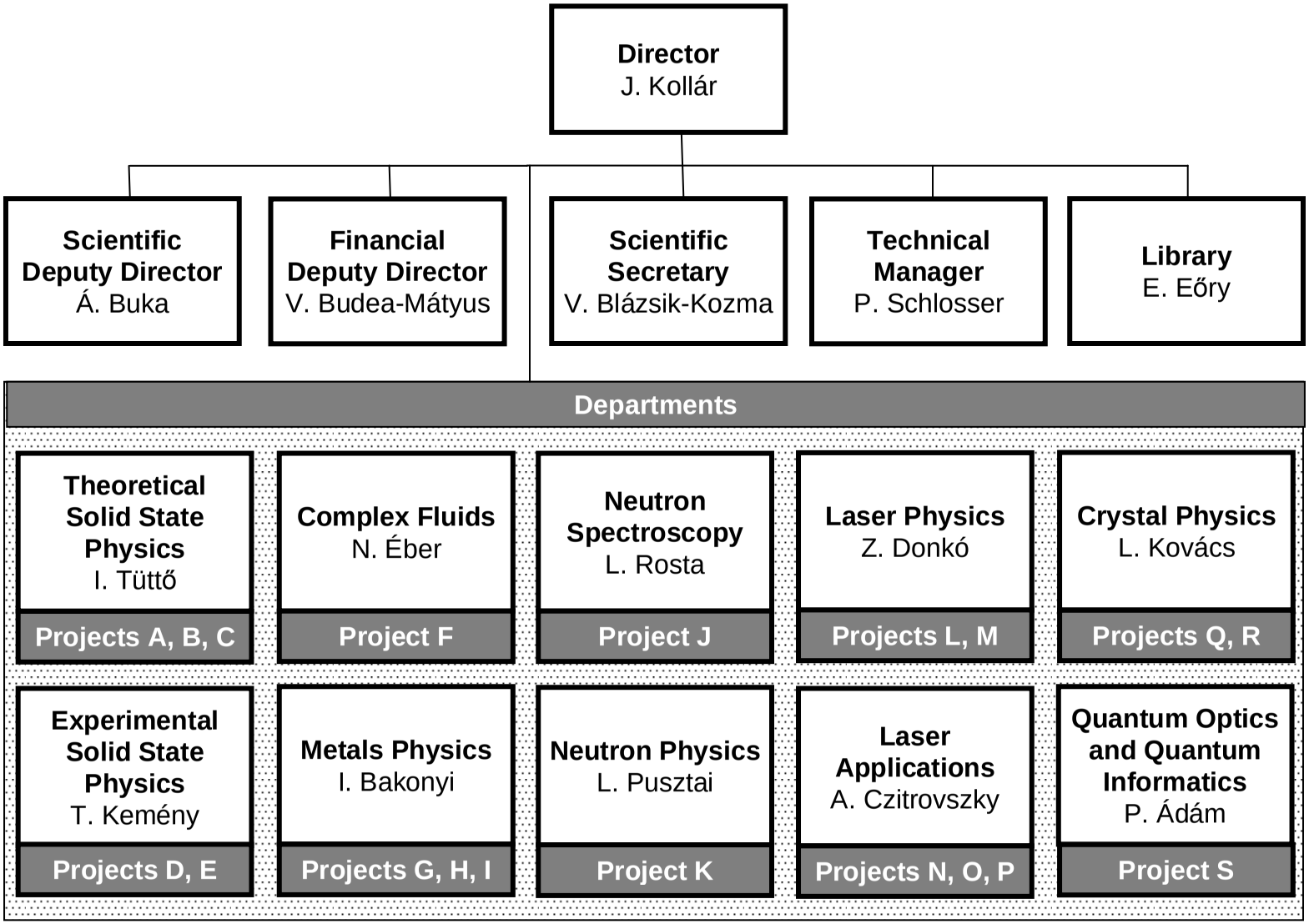
a) Sources of operation costs:



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[#], M. Lajkó[#], Ö. Legeza, K. Penc, J. Romhányi[#], E. Szirmai, K. Vladár, F. Woynarovich

Improvements of the DMRG algorithm. — The spatial topology of DMRG-based methods allows for efficient optimizations with respect to one spatial dimension only. Extending the matrix-product-state picture, we have formulated a more general approach by allowing the local sites to be coupled to more than two neighboring auxiliary subspaces. In particular, we have treated a tree-like network ansatz with arbitrary coordination number *z*. We introduced a generalized two-particle entropy function and developed a novel method which takes into account the entanglement topology of strongly correlated systems. The computational cost of the tree-tensor-network method is considerably smaller than that of previous DMRG-based procedures. In addition, we have investigated the effect of unitary transformations on the local basis states and presented a method for optimizing such transformations.

We applied this procedure to various models with long-range interactions to determine their low-energy properties. For the Hubbard model, the optimized transformation interpolates smoothly between real space and momentum space. Calculations carried out on small quantum chemical systems support our approach.

In the study of transition metal clusters we demonstrated the competition between entanglement and interaction localization. The configuration-interaction based dynamically extended active space procedure significantly reduces the effective system size and accelerates the speed of convergence for complicated molecular electronic structures. 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 on transition metal clusters. We proposed a recipe for performing DMRG calculations in a black-box fashion and we pointed out the connections of our work to other tensor network state approaches.

Exotic magnetic orders of high-spin ultracold atoms. — The Hubbard model was used to describe ultracold bosonic or fermionic atoms with spin $s > 1/2$ loaded into an optical lattice. Making convenient rearrangements of the interaction terms and exploiting their symmetry properties, low energy effective models with nearest-neighbor interactions have been derived. Applying the method to $s = 3/2$ fermions on a two-dimensional square lattice at quarter filling, we have solved the mean-field equations for repulsive singlet g_0 and quintet g_2 couplings. We have found that the plaquette state appearing in the highly symmetric SU(4) case ($g_0=g_2$) does not require fine tuning and is stable in an extended region of phase space. This phase competes with an SU(2) flux state that is always suppressed for repulsive interactions. The SU(2) flux state becomes stable in the presence of a weak applied magnetic field. For $s = 5/2$ fermions a similar SU(2) plaquette phase appears and is the ground state in the absence of external field in an extended region of the parameter space.

Frustrated magnetic systems. — Frustrated systems − e.g., frustrated antiferromagnets, where competing interactions suppress classical Néel order − are paradigms for complex behavior in condensed matter and statistical physics. In some highly frustrated magnets, spins do not order at any temperature and the resulting spin-liquid ground state retains only

[#] PhD student

short-ranged spin–spin correlations. A typical example is the classical antiferromagnet on the pyrochlore lattice, where spin correlations decay algebraically at sufficiently low temperatures; a behavior characteristic of a “Coulomb phase” arising from a strong local constraint. Extending the model to nearest-neighbor biquadratic exchange, we have shown the existence of nematic and vector-multipole orders hidden in the different Coulomb phases of the model in finite magnetic fields. Our results suggest that the magnetic properties of Cr spinels, which exhibit half-magnetization plateaux, may be largely independent of the type of magnetic order present.

Metal–insulator transitions driven by correlations and the nature of the Mott insulating phase represent one of the central themes of contemporary condensed matter physics and also of the physics of ultracold atomic gases. The canonical case of two-flavor fermions on square lattices is fully understood: for strong interactions, the ground state is an antiferromagnetically ordered two-sublattice Néel state. Recent experimental advances using multi-flavor atomic gases have paved the way to the investigation of Mott insulating states with more than two flavors in optical lattices. While it is intuitively clear that Mott insulating states will exist at particular commensurate fillings, the nature and the 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. Combining a semiclassical analysis with exact diagonalization, we have shown that the Mott insulating state of three-flavor fermions in the strong-coupling limit for one particle per site develops three-sublattice long-range order on the square lattice. This surprising pattern for a bipartite lattice with only nearest-neighbor interactions is shown to be the consequence of a subtle quantum order-by-disorder mechanism.

The projection operator approach to Heisenberg-like models provided significant results in the fields of quantum magnets. This approach was used by Majumdar and Ghosh for the s=1/2 Heisenberg chains, and Affleck, Kennedy, Lieb, and Tasaki for the s=1 Heisenberg chain to find models with exactly solvable ground states. In this spirit, we have considered a three-leg spin tube and have constructed a class of models with twofold degenerate exact ground states that break the translational symmetry. The ground states are complicated entangled states with locally resonating singlet valence bonds (this is in contrast to the Majumdar-Ghosh and AKLT models, where the valence bonds are static). As we change the parameters of the model, we find a critical point with an unusual low-energy spectrum.

The orthogonal dimer structure in the $SrCu_2(BO_3)_2$ spin-1/2 magnet provides a realization of the Shastry-Sutherland model. Using a dimer-product variational wavefunction, we have mapped out the phase diagram of the Shastry-Sutherland model including anisotropies − the Dzyaloshinskii-Moriya interaction and the g-tensor anisotropy. Based on the variational solution, we have constructed a bond-wave approach to obtain the excitation spectra as a function of magnetic field. The characteristic features of the experimentally measured neutron and ESR spectra are reproduced, like the anisotropy induced zero field splittings and the persistent gap at higher fields.

Completely integrable system. — Motivated by the fact that the O(1) corrections due to the saddle point fluctuations to the macroscopic free energy of Bethe Ansatz systems had to be completed by the contribution of an apparently ad hoc normalization of the partition function in order to reproduce the form expected on the basis of other considerations, we have revisited the calculation of the partition function for the completely integrable 1D systems. Most of the earlier calculations, following Yang and Yang, start with a partition function formulated in terms of the rapidity densities. We have shown that the precise

definition of the partition function in terms of the quantum numbers reproduces the nontrivial normalization without further considerations.

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Grants and international cooperations

OTKA[1] K68340 Quantum phase transitions in low-dimensional magnetic and fermionic systems (J. Sólyom, 2007–2011)

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

HAS-Estonian Academy of Sciences NMR and ESR studies of low dimensional strongly correlated electron systems (K. Penc, 2010-2011).

Publications

Articles

A.1. Barcza G, Legeza Ö, Gebhard[*] F, Noack[*] RM; Density-matrix renormalization-group study of excitons in polydiacetylene chains; *Phys. Rev. B;* **81**, 045103/1-11, 2010

A.2. Sikora[*] O, Pollmann[*] F, Shannon[*] N, Penc K, Fulde[*] P; Quantum liquid with delocalized fractional excitations in three dimensions; *Phys Rev Lett*; **103**, 247001/1-4, 2009

A.3. Murg[*] V, Legeza Ö, Noack[*] RM, Verstraete[*] F; Simulating strongly correlated quantum systems with tree tensor networks; *Phys. Rev. B;* **82**, 205105/1-11, 2010

A.4. Szirmai E, Lewenstein[*] M; Exotic magnetic orders for high-spin ultracold fermions; arXiv:1009.4868

A.5. Shannon[*] N, Penc K, Motome[*] Y; Nematic, vector-multipole, and plateau-liquid states in the classical O(3) pyrochlore antiferromagnet with biquadratic interactions in applied magnetic field; *Phys Rev B*; **81**, 184409/1-24, 2010

A.6. Tóth[*] TA, Läuchli[*] A, Mila[*] F, Penc K; Three-sublattice ordering of the SU(3) Heisenberg model of three-flavor fermions on the square and cubic lattices; arXiv:1009.1398

[1] OTKA: Hungarian Scientific Research Fund

[*] The author is not a member of the Research Institute for Solid State Physics and Optics staff

A.7. Romhányi J, Totsuka* K, Penc K; The effect of Dzyaloshinskii-Moriya interactions on the phase diagram and magnetic excitations of $SrCu_2(BO_3)_2$; arXiv:1010.4476

A.8. Woynarovich F; On the normalization of the partition function of Bethe Ansatz systems; arXiv:1007.1148v1

A.9. Toth* TA, Lauchli* AM, Mila* F, Penc K; Three-sublattice ordering of the SU(3) Heisenberg model of three-flavor fermions on the square and cubic lattices; *Phys Rev Lett*; accepted for publication

Conference proceeding

A.10. Szirmai E, Sólyom J; Momentum-dependent superconducting order in a one-dimensional fermion system; In: *Proc of International Conference on Magnetism, Karlsruhe, July 26-31, 2009*; *Journal of Physics: Conference Series;* **200**, 012195/1-4, 2010

Books and book chapters

A.11. Sólyom J; A modern szilárdtest-fizika alapjai. II. Fémek, félvezetők, szupravezetők (Fundamentals of the Physics of Solids, II. Metals, Semiconductors, Superconductors, in Hungarian), Eötvös Kiadó, 2010

A.12. Sólyom J; Fundamentals of the physics of solids, Vol. 3 Normal, broken-symmetry, and correlated systems; Springer, Berlin Heidelberg New York, 2010

A.13. Penc K, Läuchli* A; Spin Nematic phases in quantum spin systems; In: *Introduction to frustrated magnetism*; Springer Series in Solid-State Sciences, Vol. 164, Eds. C. Lacroix, F. Mila, and P. Mendels, Springer, accepted for publication

B. COMPLEX SYSTEMS

F. Iglói, R. Juhász, I. Kovács[#], N. Menyhárd, 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. — The infinite disorder fixed point of the random transverse-field Ising model is expected to control the critical behavior of a large class of random quantum and stochastic systems having an order parameter with discrete symmetry. We have studied this model on the square lattice with a very efficient numerical implementation of the strong disorder renormalization group method, which makes us possible to treat finite samples of linear size up to L = 2048. We have calculated sample dependent pseudo-critical points and studied their distribution, which is found to be characterized by the same shift and width exponent: $\nu = 1.24(2)$. For different types of disorder the infinite disorder fixed point is shown to be characterized by the same set of critical exponents, for which we have obtained improved estimates: $x = 0.982(15)$ and $\psi = 0.48(2)$. We have also studied the scaling behavior of the magnetization in the vicinity of the critical point as well as dynamical scaling in the ordered and disordered Griffiths phases.

We have studied diffusion of a particle in a system composed of K parallel channels, where the transition rates within the channels are quenched random variables whereas the inter-channel transition rate v is homogeneous. A variant of the strong disorder renormalization group method and Monte Carlo simulations are used. Generally, we have observed anomalous diffusion, where the average distance travelled by the particle, $[x(t)]_{av}$, has a power-law time-dependence $[x(t)]_{av} \sim t^{\mu_K(v)}$, with a diffusion exponent $0 \leq \mu_K(v) \leq 1$. In the presence of left-right symmetry of the distribution of random rates the recurrent point of the multi-channel system is independent of K, and the diffusion exponent is found to increase with K and decrease with v. In the absence of this symmetry, the recurrent point may be shifted with K and the current can be reversed by varying the lane change rate v.

Quenched disorder is known to play a relevant role in dynamical processes and phase transitions. Its effects on the dynamics of complex networks have hardly been studied. Aimed at filling this gap, we have analyzed the contact process, i.e. the simplest propagation model, with quenched disorder on complex networks. We have found Griffiths phases and other rare region effects, leading rather generically to anomalously slow (algebraic, logarithmic, etc.) relaxation, on Erdős-Rényi networks. Similar effects are predicted to exist for other topologies with a finite percolation threshold. More surprisingly, we have found that Griffiths phases can also emerge in the absence of quenched disorder, as a consequence of topological heterogeneity in networks with finite topological dimension. These results have a broad spectrum of implications for propagation phenomena and other dynamical processes on networks.

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

[#] PhD student

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 shown that spin and fermion representations for solvable quantum chains lead in general to different reduced density matrices if the subsystem is not singly connected. We have studied the effect for two sites in XX and XY chains as well as for sublattices in XX and transverse Ising chains.

Trapped superfluid Fermi gas has been investigated on the BCS side of the Feshbach resonance using the Green's function technique. At the Feshbach resonance the universal prefactor has been derived for the von Weizsäcker type correction to the local density approximation.

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Péter Szépfalusy	psz@szfki.hu

Grants and international cooperations

OTKA T075324	Effects of disorder in many body systems (F. Iglói, 2009-2012)
OTKA K77629	Investigation of fundamental problems of phase transitions and symmetry breaking phases (P. Szépfalusy, 2009-2012)
HAS-DFG/193	Statistical physics of disordered systems (F. Iglói, 2008-2009)

Publications

Articles

B.1. Kovács IA, Iglói F; Critical behavior and entanglement of the random transverse-field Ising model between one and two dimensions; *Phys Rev B*; **80**, 214416/1-9, 2009

B.2. Iglói F, Peschel* I; On reduced density matrices for disjoint subsystems; *EPL*; **89**, 40001/1-6, 2010

B.3. Juhász R, Iglói F; Anomalous diffusion in disordered multi-channel systems; *J Stat Mech*; P03012/1-17, 2010

B.4. Kovács IA, Iglói F; Renormalization group study of the two-dimensional random transverse-field Ising model; *Phys Rev B*; **82**, 054437/1-13, 2010

B.5. Karsai* M, Anglès d'Auriac* J-Ch, Iglói F; Interface mapping in two-dimensional random lattice models; *J Stat Mech*; P08027/1-14, 2010

B.6. Juhász R; Dynamics at barriers in bidirectional two-lane exclusion processes; *J Stat Mech*; P03010/1-23, 2010

B.7. Munoz* MA, Juhász R, Castellano* C. Ódor* G; Griffiths phases on complex networks; *Phys Rev Lett*; **105**, 128701/1-4, 2010

B.8. Csordás* A, Almásy* O, Szépfalusy P; Gradient corrections to the local density approximation for trapped superfluid Fermi gases; *Phys Rev A*; accepted for publication

See also: E.20.

C. ELECTRONIC STATES IN SOLIDS

J. Kollár, T. Demjén[#], Á. Gali, K. Kádas, B. Lazarovits, E. Simon[#], I. Tüttő, B. Újfalussy, A. Virosztek[+], L. Vitos, V. Zólyomi

The phase stability of group VB (V, Nb, and Ta) transition metals is explored by **first-principles electronic-structure calculations**. Alloying with a small amount of a neighboring metal can either stabilize or destabilize the body-centered-cubic phase relative to low-symmetry rhombohedral phases. We show that band-structure effects determine phase stability when a particular group VB metal is alloyed with its nearest neighbors within the same d-transition series. In this case, the neighbor with less (to the left) and more (to the right) d electrons destabilize and stabilize bcc, respectively. When alloying with neighbors of higher d-transition series, electrostatic Madelung energy dominates and stabilizes the body-centered-cubic phase. This surprising prediction invalidates current understanding of simple d-electron bonding that dictates high-symmetry cubic and hexagonal phases.

The third element effect to improve the high temperature corrosion resistance of the low-Al Fe-Cr-Al alloys is suggested to involve a mechanism that boosts the recovering of the Al concentration to the required level in the Al-depleted zone beneath the oxide layer. We propose that the key factor in this mechanism is the coexistent Cr depletion that helps to maintain a sufficient Al content in the depleted zone. Several previous experiments related to our study support that conditions for such a mechanism to be functional prevail in real oxidation processes of Fe-Cr-Al alloys.

***Ab initio* electronic-structure methods** are used to study the properties of $Fe_2P_{1-x}Si_x$ in ferromagnetic and paramagnetic states. The calculated lattice parameters, atomic positions, and magnetic properties are in good agreement with the experimental and other theoretical results. In contrast to the observation, for the ferromagnetic state the body centered orthorhombic structure (bco, space group *Imm*2) is predicted to have lower energy than the hexagonal structure (hex, space group *P*62*m*). The zero-point spin fluctuation energy difference is found to be large enough to stabilize the hex phase. For the paramagnetic state, the hex structure is calculated to be the stable phase and the computed total energy versus composition indicates a hex to bco crystallographic phase transition with increasing Si content. The phonon vibrational free energy, estimated from the theoretical equation of state, turns out to stabilize the hexagonal phase, whereas the electronic and magnetic entropies favor the low symmetry orthorhombic structure.

The composition-dependent lattice parameters and elastic constants of $In_{1-x}Tl_x$ ($0<x<0.4$) alloy in face-centered-cubic (fcc) and face-centered-tetragonal (fct) crystallographic phases are calculated by using the **first-principles exact muffin-tin orbitals (EMTO) method** in combination with coherent-potential approximation. The calculated lattice parameters and elastic constants agree well with the available theoretical and experimental data. For pure In, the fcc phase is mechanically unstable as shown by its negative tetragonal shear modulus *C*'. With Tl addition, *C*' of the fcc phase increases whereas that of the fct phase decreases, indicating that the fcc phase becomes mechanically more stable and the fct phase becomes less stable. In addition, the structural energy difference between the fcc and fct phases decreases with *x*. Both of these effects account for the observed lowering of the fcc-fct martensitic transition temperature upon Tl addition to In. The G43

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density of states indicates that the stability of the fct phase relative to the fcc one at low temperatures is due to the particular electronic structure of In and In-Tl alloys.

The structure and the composition of the **Earth's solid inner core** are still unknown. Iron is accepted to be the main component of the core. Based on EMTO studies, we described the elastic properties of hexagonal closed-packed (hcp) Fe-Mg alloys, containing 5 and 10 atomic % Mg, up to pressures of the Earth's inner core. We demonstrated the effect of Mg alloying on the hexagonal axial ratio, elastic constants, density and sound wave velocities, and show that the shear modulus and the transverse sound velocity of hcp Fe are notably reduced by Mg. Though the calculated shear moduli and sound velocities of hcp Fe-Mg alloys still differ significantly from those of the core as provided by seismic observations, even at 10% Mg content, Mg alloying changes the elastic properties of hcp iron in such a way that the differences to the seismic data decrease. At core conditions, we predicted that 5-10% Mg stabilizes the body-centered-cubic (bcc) phase of Fe both dynamically and thermodynamically, and we gave an electronic structure explanation of this phenomenon. We demonstrated that the physical properties of bcc Fe-Mg alloys containing 5-10% Mg reproduce those of the inner core: the calculated density, elastic moduli and sound velocities of bcc Fe-Mg alloys are consistent with seismic data. Therefore the bcc-structured Fe-Mg alloy seems to be amongst the strongest candidate models for the Earth's solid inner core.

By means of first principles density functional theory, we investigated the properties of **TiN/Fe interfaces**, namely the TiN(001)/fcc Fe(111) and TiN(001)/bcc Fe(110) interfaces. We demonstrated that along certain directions Fe slides with negligible energy barriers against TiN at both interfaces, whereas sliding along other directions is involved with significant energy barriers. The interface between bcc Fe and TiN has a low energy barrier for sliding along the [110] direction of the TiN lattice, as does sliding along the [010] direction at TiN(001)/fcc Fe(111). For fcc Fe on TiN, a large energy barrier is found for sliding along the [100] direction of the TiN lattice. We showed that this phenomenon and the stability of these interfaces are determined by the interplay between N-Fe bonding and Ti-Fe antibonding interactions.

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. They include a comprehensive study of the binding of transition metals on graphene (which is relevant for single molecule sensing and single atom mass sensing applications), a study of the so-called quantum pumping effect with double-walled carbon nanotubes (including proposing a design for a specific nanotube-based quantum pump which could be used as an energy scavenger to power National Energy Modeling System), a study of the Raman signal of fullerene-nanotube peapods in electrochemistry (which have shown that a small charge penetrates the nanotube wall and occupies the fullerenes), a study of the so-called bamboo defects in the inner shell of peapod-grown double-walled carbon nanotubes (which should motivate experimental studies of electron transport through such structures), and a study of the anomalous behavior of the D* Raman band of double-walled carbon nanotubes (which points out the importance of curvature at low diameters).

We explored the strong variations of the **electronic properties of copper-oxigen compounds** across the doping phase diagram in a quantitative way. We calculated the electronic Raman response on the basis of results from angle-resolved photoemission spectroscopy (APRES). In the limits of our approximations we found agreement on the overdoped side and pronounced discrepancies at lower doping. In contrast to the

successful approach for the transport properties at low energies, the Raman and the APRES data cannot be reconciled by adding angle-dependent momentum scattering.

In the front of biomarkers the group has important results on **silicon carbide (SiC) nanoparticles** (A1). SiC nanoparticles are very promising candidates to realize bioinert luminescent quantum dots that might be safely used *in vivo* for detecting biological molecules. It is crucial to understand the optical properties of these SiC nanoparticles. We showed by time-dependent density functional calculations that double bonds between carbon and oxygen present at the surface can significantly influence the absorption spectrum of the entire SiC nanoparticles by reducing the optical gap by a few electronvolts. This result can explain some controversial experimental data on the excitation spectrum of SiC nanoparticles fabricated with different techniques. Our result can guide the growers and experimentalists how to control the optical properties of SiC nanoparticles. We showed this result at the 8th European Conference of Silicon Carbide and Related Materials.

As a continuation of the research in relation to **surface RKKY interactions** we studied the interaction between impurities on alloy surfaces using first principles calculations. We showed that there is at least three different mechanism for the impurities to interact. On surfaces where there is a surface state, the interaction shows an oscillatory behaviour similarly to bulk, and the frequency of oscillation depends on the Fermi vector of the surface state. This property becomes interesting when the (111) surface of a CuPd alloy is studied. As the Pd concentration increases, the Fermi surface closes the L-gap, the surface state disappears at about 18% of Pd concentration. With the disappearance of the surface state the oscillatory interaction of surface magnetic impurities gives place to an exponentially decaying one. However, on the Pd rich side, the oscillatory interaction reappears, with a bulk RKKY frequency, suggesting a different mechanism. It is found that this mechanism is based on the bulk-like interaction of induced moments well beneth the surface of the alloy.

We investigated the properties of **interacting electrons possessing an ultrarelativistic (conical) Dirac spectrum**. In solids these are to be found in at least two places. A certain type of unconventional density wave (UDW) is thought to be the competing ground state in the pseudogap phase of underdoped high-T_c superconductors (SC). We studied theoretically the optical and Raman response of such system of coexisting UDW and SC in the presence of randomly distributed impurities. We found that in addition to the SC condensate, the UDW condensate also contributes to the Raman scattering intensity. The other system with Dirac spectrum is graphene. We calculated the critical properties of an antiferromagnetic phase transition due to repulsive interaction between electrons having density of states (DOS) linear in energy. We found finite critical interaction and unconventional critical exponents. We extended our analysis to systems where the DOS has a general power law dependence on energy. We also described in detail both the long and the short wavelength pattern in the local DOS and Friedel oscillations around a well localized impurity in graphene.

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Grants and international cooperations

OTKA T046267 Complex analysis of magnetic nanostructure for high density recording (B. Újfalussy, 2007-2010)

OTKA F68726 The consequences of the electron localization on the electronic structure and magnetic properties of surface nanostructures (B. Lazarovits, 2007-2010)

OTKA F68852 Theoretical investigation of inter-molecular interactions in nanostructures (V. Zólyomi, 2007-2010)

HAS Momentum program, New theoretical spectroscopy group in the Research Institute for Solid State Physics and Optics: design and characterization of semiconductor nanostructures for biomarker, solar cell and magnetometer application (Á. Gali. 2010-2013)

National Science Fund 1035468, SOLAR Collaborative: Multiple exciton generation and charge extraction in all-Inorganic nanostructured solar cells (G. Zimanyi, USA, 2010-2013, SZFKI participant: Á. Gali)

STINT Swedish-Hungarian joint project, Atomic-scale investigation of steel materials by first principles method (L. Vitos, 2009-2011)

Publications

Articles

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C.37. Oroszlány* L, Zólyomi V, Lambert* C J; Carbon nanotube Archimedes screws; *ACS Nano*, accepted for publication

C.38. Zólyomi V, Rusznyák* Á, Kürti* J, Lambert* C J; First principles study of the binding of 4d and 5d transition metals to graphene; *J Phys Chem C*; accepted for publication, DOI: 10.1021/jp107669b, 2010

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Book chapter

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D. NON-EQUILIBRIUM ALLOYS

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

Sequence permutation of three building block multilayers was recently suggested as a new approach in studying bottom and top interfaces formed of a given layer with either of the other two elements. The layer permutation, however, may influence the sample morphology to a large extent, as it was revealed by transmission electron microscopy investigations in case of Fe-B-Ag multi-trilayers. Large interface roughness and waviness of the layers was observed when Ag was grown on top of the B layer, but B was found to grow on Ag smoothly. The Fe-Ag and Fe-B interfaces did not show such a large difference. As a consequence of the above interface properties, the variance of the Ag layer thickness was larger for the Fe/B/Ag than for the B/Fe/Ag sequence. From comparison of Mössbauer measurements on trilayer and multilayer samples the following conclusions have been drawn. In case of the B/Fe/Ag sequence the 5 nm nominal thickness Ag layers applied could be supposed to act as barriers to the diffusion between the Fe and B layers separated by them, but in case of the Fe/B/Ag sequence the variance of the Ag layer thickness allowed the mixing between them to a measurable extent. To study in more details how the thickness of the Ag layers interleaved into Fe-B multilayers influences the chemical mixing of Fe and B the following samples were prepared and studied:

Si / 5 nm Ag / [2 nm B / 2 nm ^{57}Fe / x nm Ag]$_4$ / cover layer, x=0.2, 0.4, 1, 2, 4, 5 and 10.

The changes observed for varying Ag layer thickness can be understood if we suppose that below 5 nm nominal thickness the Ag layer is not continuous, as it is illustrated in Fig. 1.

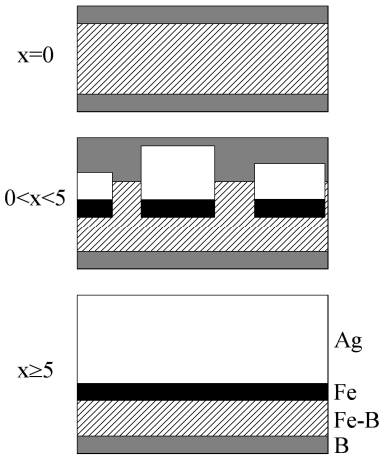

Fig. 1 *Schematic sample structures formed by interface mixing in case of different thickness of the Ag layer in the [2 nm B / 2 nm ^{57}Fe / x nm Ag]$_4$ multilayer series, as inferred from the Mössbauer measurements. In case of a continuous Ag layer (x≥5) mixing of Fe and B (dashed area) takes place only at the bottom side of the Fe layer. When there is no Ag layer interleaved (x=0), it occurs both at the bottom and the top sides and the 2 nm Fe layer is fully amorphized. For 0<x<5 Ag islands are formed with varying area and height and protect the top side of the underlying Fe area from amorphization.*

The trends observed in the hyperfine fields (HFs) of the amorphous Fe-B interfaces are in accordance with the result obtained from the sequence permutation studies: the average HF is larger (i.e. the average B concentration is smaller) when the ratio of the bottom (B/Fe) interfaces is larger in the sample.

When the thickness of the Fe layers is reduced to 1 nm all the Fe atoms are involved in interface mixing. The Ag layers become continuous also at about 5 nm thickness and the magnetic properties become insensitive to the Ag thickness. The average Fe concentration of the amorphous Fe-B layer is more than 60 at% and the ultra-thin amorphous layers sandwiched in between amorphous B and crystalline Ag, as shown in Fig. 2, have good ferromagnetic properties.

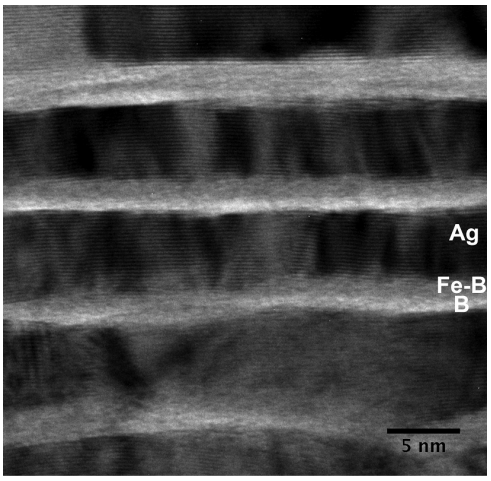

Fig. 2 *High resolution transmission electron microscopy image of the [1 nm B/ 1 nm Fe/ 10 nm Ag]$_5$ multilayer.*

Influence of Mn on the magnetocaloric effect of Nanoperm-type alloys. — The influence of the Mn content on the magnetocaloric response of ribbon-shaped amorphous samples of $Fe_{80-x}Mn_xB_{20}$ (x=10, 15, 18, 20 and 24), has been studied. For this purpose, the temperature and field dependence of the magnetic entropy change (ΔS_M) have been obtained from magnetization curves. The partial substitution of Fe by Mn leads to a monotonous change of the Curie temperature (T_C) of the alloys from 438 K for x=10 to 162 K for x=24, in agreement with the coherent-potential approximation (CPA). These Curie temperatures could make them good candidates to be used for magnetic refrigeration at room temperature. For an applied field of 1.5 T the maximum entropy change (ΔS_M^{peak}) passes from 1 $J \cdot K^{-1} \cdot kg^{-1}$ (x=10) to 0.5 $J \cdot K^{-1} \cdot kg^{-1}$ (x=24), and the refrigerant capacity (RC) varies between 117 $J \cdot kg^{-1}$ (x=10) and 68 $J \cdot kg^{-1}$ (x=24). A linear relationship between ΔS_M^{peak} and the average magnetic moment per transition metal atom ($<\mu>_{Fe,Mn}$) has been presented.

Study of Zr-alloys for nuclear reactors. — Zr-based alloy tubes are used in nuclear reactors as fuel element containers. The container material used in the Paks Nuclear Power Station is to be replaced and the Atomic Energy Institute of the Hungarian Academy of Sciences started a special program to test the new alloy. We were invited to contribute with a study of the high temperature phase transition of the new material. Heat flux calorimetry and thermo-mechanical studies were carried out by Setaram instruments in the 600-1200 K temperature range at the Material Physics Department of the Eötvös University. The traditional E110 alloy was compared with the new E110G alloy and with pure elemental Zr which also shows the phase transition. The use of the investigated new material in the very critical nuclear application was approved by our results.

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Grants and cooperations

OTKA K68612	Magnetic anisotropy of structures with reduced dimension (L.F. Kiss, 2007-2010)
269/AEKI	Study of Zr-alloys for nuclear reactors (T. Kemény, 2010)

Long term visitor

— Rafael Caballero Flores, University of Sevilla, Spain, from 26 September to 21 November, 2010 (host: L.F.Kiss)

Publications

Articles

D.1. Kiss LF, Balogh J, Bujdosó L, Kaptás D, Tanczikó* F, Vincze I; Temperature dependence of the high-field magnetization in Fe-Ag granular alloys and discontinuous multilayers; *J Phys: Conference Series*; **200**, 072050/1-4, 2010

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D.6. 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*; accepted for publication

D.7. Kiss LF, Balogh J, Bujdosó L, Kaptás D, Kemény T, Kovács* A, Vincze I; Amorphous Fe-B alloys in B-Fe-Ag multilayers studied by magnetization and Mössbauer measurements; *J All Comp*; accepted for publication

E. X-RAY DIFFRACTION

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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. In the group of A_xC_{60} compounds (A=Na, K, Rb, Cs) there are materials with interesting properties. 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. Our major activity concerns the development of this family of materials. This year we have prepared further members of the rotor-stator crystals and tried to extend the family with various V and Y shaped stator molecules. In an international collaboration we finished a complex X-ray diffuse scattering and inelastic neutron scattering study on the dynamics of $C_{60}{\cdot}C_8H_8$.

Carbon nanotubes and graphene.— This year the Nobel prize in physics was awarded for the study of graphene. We also studied carbon nanotube systems and graphene.

We concentrated on hybrid materials, composed of carbon nanotubes and other organic species, among them fullerenes. The structure of these multicomponent materials varies from chemically functionalized nanotubes to tubes filled with other molecules ("peapods") or flat molecules covering the surface of the nanotubes and establishing π-π interaction. The spectroscopy of the latter can be described in a similar way as molecules adsorbed on surfaces. We characterized such surface-bonded conducting polymers on carbon nanotubes by infrared and Raman spectroscopy. For the filled nanotubes, we optimized the procedure of filling by supercritical carbon dioxide and also developed a spectroscopic method to decide if the guest molecule is inside or outside the tubes. We performed a systematic investigation of filling nanotubes by fullerenes and then converting these fullerenes into an

[#] Ph.D. student

inside tube, to form double-walled carbon nanotubes (DWNT's). We continued the study of other supramolecular structures by vibrational spectroscopy, specifically, the identification of hydrogen bonds by the temperature and concentration dependence of infrared spectra, and the assignment of the vibrations in cooperation with theorists using molecular dynamics calculations. We also made further progress on graphene, performing Raman spectroscopy on samples which have been patterned by chemical or litographic methods**.**

Theory of phase transformations. — A simple dynamical density functional theory, the phase-field crystal (PFC) model, was used to describe homogeneous and heterogeneous crystal nucleation in two-dimensional monodisperse colloidal systems and crystal nucleation in highly compressed Fe liquid. External periodic potentials were used to approximate inert crystalline substrates in addressing heterogeneous nucleation. In agreement with experiments in 2D colloids, the PFC model predicts that in 2D supersaturated liquids, crystalline freezing starts with homogeneous crystal nucleation without the occurrence of the hexatic phase. At extreme supersaturations, crystal nucleation happens after the appearance of an amorphous precursor both in two and three dimensions. Contrary to expectations based on the classical nucleation theory, it is shown that corners are not necessarily favorable places for crystal nucleation. Finally, it is shown that by adding external potential terms to the free energy, the PFC theory can be used to model colloid patterning experiments.

The PFC model has been used to address polymorphism, crystal nucleation, and crystal growth in the diffusion-controlled limit. We have refined the phase diagram of the PFC model in 3D, determined the line free energy in 2D and the height of the nucleation barrier in 2D and 3D for homogeneous and heterogeneous nucleation. We have demonstrated that, in the PFC model, bcc, fcc, and hcp structures compete, while the simple cubic structure is unstable, and that phase preference can be tuned by changing the model parameters: Close to the critical point the bcc structure is stable, while far from the critical point the fcc prevails, with an hcp stability domain in between. With increasing distance from the critical point the equilibrium crystal shapes vary from sphere to specific faceted shapes: rhombic dodecahedron (bcc), truncated octahedron (fcc), and hexagonal prism (hcp). The growth rate has been found time dependent and anisotropic; an anisotropy that depends on the driving force. It has been shown that due to the diffusion-controlled growth mechanism, relevant to crystal aggregation in colloidal systems, dendritic structures evolve in large-scale isothermal PFC simulations. An oscillatory effective pair potential resembling those proposed for model glass formers has been evaluated from structural data of the amorphous phase obtained by instantaneous quenching. We have explored eutectic solidification in a binary PFC model.

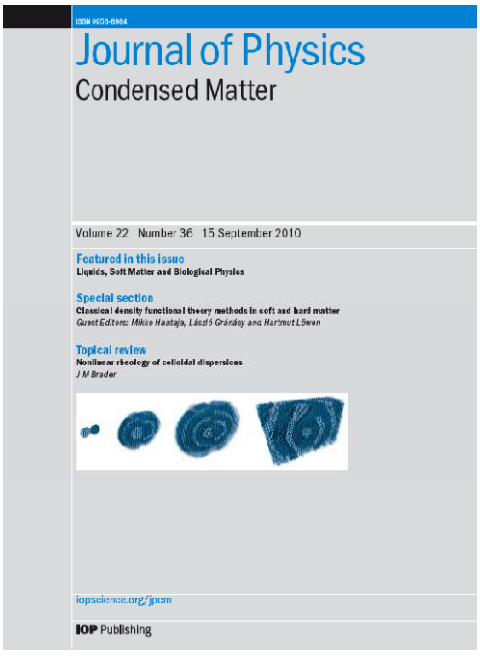

Fig. 1 *Eutectic solidification as predicted by the binary phase-field crystal simulation: Cover page of a special issue of the J. Phys.: Condens. Matter.*

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Grants and international cooperations

OTKA K062588 Dynamics of complex systems (T. Pusztai, 2006-2011)

OTKA K 72954 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 NI 67842 Experimental and theoretical investigation of carbon nanostructures (K. Kamarás, 2007-2010)

OTKA T 075813 Polymerization in carbon nanostructures (K. Kamarás, 2009-2012)

OTKA K 67866 Development and application of local methods in solid state physics, (G. Faigel, 2007-2010)

OTKA K-81348 Ultrafast diffraction imaging of single particles (M. Tegze, 2010-2014)

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)

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)

EU FP6-Marie Curie Research Training Network MRTN-CT-2006-035810: Supramolecular hierarchical self-assembly of organic molecules onto surfaces towards bottom-up nanodevices: a host-driven action (PRAIRIES) (coordinator: Francois Diederich, ETH Zürich, Switzerland, representative of Contractor: K. Kamarás, 2006-2010)

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: Nicola Armaroli, CNR-ISOF, Bologna, Italy, representative of contractor: K. Kamarás, 2008-2012)

FP7 PRE-XFEL 211604 Preparatory phase of the european X-ray free electron laser facility (G. Faigel, 2008-2011)

Long term visitor

— Alban Etchevers, undergraduate student, Ecole Polytechnique Universitaire de Grenoble, France; June 1 - August 20, 2010 (host: S. Pekker)

Publications

Articles

E.1. Kamarás K, Botka B, Pekker Á, Ben-Valid* S, Zeng* A, Reiss* L, Yitzchaik* S; Surface-induced changes in the vibrational spectra of conducting polymer - carbon nanotube hybrid materials; *Phys Stat Sol (b)*; **246**, 2737-2739, 2009

E.2. Abouelsayed* A, Thirunavukkuarasu* K, Kamarás K, Hennrich* F, Kuntscher* CA; Pressure-induced phenomena in single-walled carbon nanotubes probed by infrared spectroscopy*; High Pressure Res;* **29**, 559-563, 2009

E.3. Haataja* M, Gránásy L, Löwen* H; Classical density functional theory methods in soft and hard matter; *J Phys: Condens Matter;* **22**, 360301/1–8, 2010

E.4. Tóth GI, Tegze G, Pusztai T, Tóth* G, Gránásy L; Polymorphism, crystal nucleation and growth in the phase-field crystal model in 2d and 3d; *J Phys: Condens Matter;* **22**, 364101/1–17, 2010

E.5. Bousige* C, Rols* S, Cambedouzou* J, Verberck* B, Pekker S, Kováts É, Durkó* G, Jalsovszky* I, Pellegrini* É, Launois* P; Lattice dynamics of a rotor-stator molecular crystal: Fullerene-cubane $C_{60}\cdot C_8H_8$, *Phys Rev B*; **82**, 195413/1-10, 2010

E.6. Nemes-Incze* P, Magda* G, Kamarás K, Bíró* LP; Crystallographic orientation dependent etching of graphene layers; *Phys Stat Sol (c);* 7, 1241-1245, 2010

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E.8. Pekker Á, Kamarás K; A general figure of merit for thick and thin transparent conductive carbon nanotube coatings; *J Appl Phys;* **108**, 054318/1-7, 2010

E.9. Thirunavukkuarasu* K, Hennrich* F, Kamarás K, Kuntscher* CA; Infrared spectroscopic studies on unoriented single-walled carbon nanotube films under hydrostatic pressure; *Phys Rev B;* **81**, 045424/1-12, 2010

E.10. Müller* M, Meinke* R, Maultzsch* J, Syrgiannis* Z, Hauke* F, Pekker Á , Kamarás K, Hirsch* A, Thomsen* C; Electronic properties of propylamine-functionalized single-walled carbon nanotubes; *Phys Chem Chem Phys;* **11**, 2444-2448, 2010

E.11. Nemes-Incze* P, Magda* G, Kamarás K, Biró* LP; Crystallographically selective nanopatterning of graphene on SiO_2; *Nano Research;* **3**, 110-116, 2010

E.12. Francis* EA, Scharinger* S, Németh K, Kamarás K, Kuntscher* CA; Investigation of the Jahn-Teller effect in the C_{60}^- monoanion under high pressure; *Phys Stat Sol (b)*; accepted for publication, DOI: 10.1002/pssb.201000201

E.13. Németh K, Pekker Á, Borondics F, Jakab E, Nemes* NM, Kamarás K, Pekker S; Infrared spectra of hydrogenated HiPCo nanotubes; *Phys Stat Sol (b)*; accepted for publication, DOI: 10.1002/pssb.201000329

E.14. Botka* B, Pekker Á, Botos* Á, Kamarás K, Hackl* R; A systematic study of optical and Raman spectra of peapod-based DWNTs; *Phys Stat Sol (b)*; accepted for publication, DOI: 10.1002/pssb.201000293

E.15. Botos* Á, Khlobystov* AN, Botka* B, Hackl R, Székely* E, Simándi* B, Kamarás K; Investigation of fullerene encapsulation in carbon nanotubes using a complex approach based on vibrational spectroscopy; *Phys Stat Sol (b)*; accepted for publication, DOI: 10.1002/pssb.201000375

E.16. Tóháti HM, Botka* B, Németh K, Pekker Á, Hackl* R, Kamarás K; Infrared and Raman investigation of carbon nanotube-polyallylamine hybrid systems; *Phys Stat Sol (b)*; accepted for publication, DOI: 10.1002/pssb.201000435

E.17. Kamarás K, Pekker Á, Botka B, Hu* H, Niyogi* S, Itkis* ME, Haddon* RC; The effect of nitric acid doping on the optical properties of carbon nanotube films; *Phys Stat Sol (b)*; accepted for publication, DOI: 10.1002/pssb.201000733

E.18. Gránásy L, Tegze G, Tóth GI, Pusztai T; Phase-field crystal modelling of crystal nucleation, heteroepitaxy and patterning; *Philos Mag*; accepted for publication, DOI: 10.1080/14786435.2010.487476.

E.19. Tegze G, Gránásy L, Tóth GI, Douglas* J F., Pusztai T; Tuning the structure of non-equilibrium soft materials by varying the thermodynamic driving force for crystal ordering; *Soft Matter;* accepted for publication.

Conference proceedings

E.20. Oszlányi G, Sütő A; Missing data in a modified charge-flipping algorithm; Lecture at the *26th European Crystallographic Meeting, Darmstadt, 29 August - 2 September 2010*; Acta Cryst A; **66**, s107, 2010

E.21. Pekker Á, Kamarás K, Nemes* NM, Garcia-Hernandez* M; A figure of merit for transparent conducting nanotube films; in: *Nanotubes and Related Nanostructures — 2009, Materials Research Society Fall Meeting 2009, Boston, MA, USA, Nov 30 – Dec 4, 2009*; edited by Yoke Khin Yap (Mater. Res. Soc. Symp. Proc. Volume 1204, Warrendale, PA, 2010); 1204-K10-41, 2009

Book chapter

E.22. Klupp G, Kamarás K; Following Jahn-Teller distortions in fulleride salts by optical spectroscopy; In: *The Jahn-Teller effect: Advances and Perspectives*, Ed: Köppel H, Yarkony DR, Barentzen H, Springer Series in Chemical Physics; Vol 97, pp. 489-516, 2009

F. COMPLEX FLUIDS

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

Synthesis. — New non-symmetrical bent-core mesogens with a variable flexible chain length have been synthesized. The compounds were derived from 3-hydroxybenzoic acid, which is the central unit of the molecules. The tails on both ends were connected by ester functionality, one tail contains a terminal double bond and the other is saturated. The compounds represent novel non-symmetric molecules both in their core and tails. The main features of differential scanning calorimetry, polarizing optical microscopy, electro-optical and polarization current measurements for all studied materials indicate a transition between a single tilted synclinic ferroelectric and an antiferroelectric smectic phase.

Electric field driven pattern formation. — Two electroconvection (EC) pattern morphologies - a cellular and a subsequent roll pattern - have been detected in the same frequency range in a nematic with positive permittivity and conductivity anisotropies. The frequency dependences of the onset voltages and critical wave numbers have been determined both for homeotropic and planar alignments. It has been proven that both pattern morphologies have a dielectric time symmetry. Possible sources for the pattern formation in the frame of both the isotropic Felici-Benard mechanism, as well as the standard model of EC have been considered.

A binary system made of bent-core and calamitic nematic liquid crystals has been studied by dielectric spectroscopy. The pure bent-core nematic exhibited two more dispersions than expected. Some dispersions occurred at unusually low frequencies, both in the nematic and the isotropic phases. It has been shown that the frequency dependent dielectric properties of the binary mixtures can be explained as a superposition of the dispersions of its constituents. The signs of the permittivity and conductivity anisotropies agree with those expected from the electroconvection morphologies.

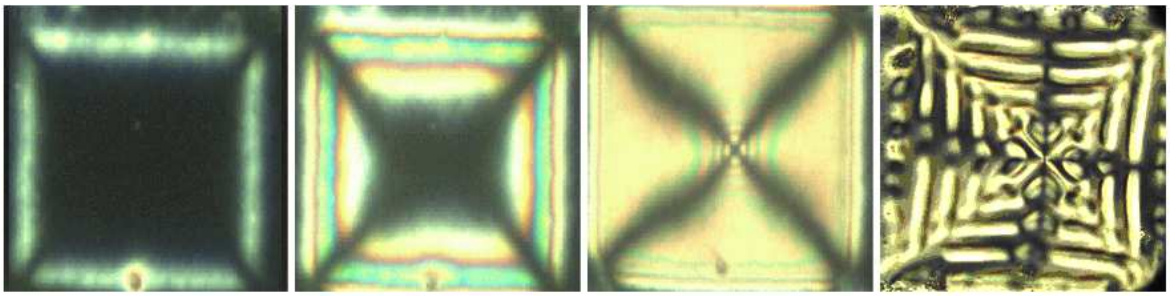

***Fig. 1** Director distortion at increasing voltages.*

Director reorientation by electric and magnetic fields has been studied at electrode sizes comparable with cell thicknesses (see Fig. 1). It was found that reorientation starts at the electrode edges at lower voltages than in extended samples due to the field inhomogeneity. The symmetry of the deformation was broken by an additional magnetic field. Numerical simulation of the director field and the resulting birefringence has been carried out, resulting in a good agreement with the experiments.

[#] Ph.D. student

Liquid crystal composite materials. — Ferronematic liquid crystals of low negative anisotropy of the diamagnetic susceptibility have been prepared by doping the liquid crystal with magnetic Fe_3O_4 particles. High magnetic fields were applied perpendicular to, or parallel with the initial director. The observed structural instabilities have been interpreted within the Burylov and Raikher's theory. Using capacitance measurements, the Freedericksz threshold magnetic field of the ferronematic B_{FN}, and the critical magnetic field B_{max}, at which the initial parallel orientation between the director and the magnetic moment of magnetic particles breaks down, have been determined. The values of these quantities have been used to estimate the surface density of the anchoring energy W of liquid crystal molecules on the surface of the magnetic particles. The obtained values indicate a soft anchoring of the liquid crystal on the magnetic particles with a preferred parallel orientation of the magnetic moment of magnetic particles with the director.

Granular dynamics. — Shearing a granular material often leads to shear localization, where the region with the highest shear rate called shear zone usually finds the shortest way through the material. In an inhomogeneous (e.g., layered) system, where different regions (layers) are characterized with different effective friction, a more complicated trajectory will develop. When increasing the load on a layered system initially at rest, the zone will appear along that path which corresponds to the minimal resistance of the system (principle of "the easiest bond breaks"). This is similar to the well known Fermat's principle in optics, where the optimal trajectory of a light beam results from the minimization of the optical path. We have shown that in the granular system the shear zone can be refracted at the layer boundary, analogously to light refraction.

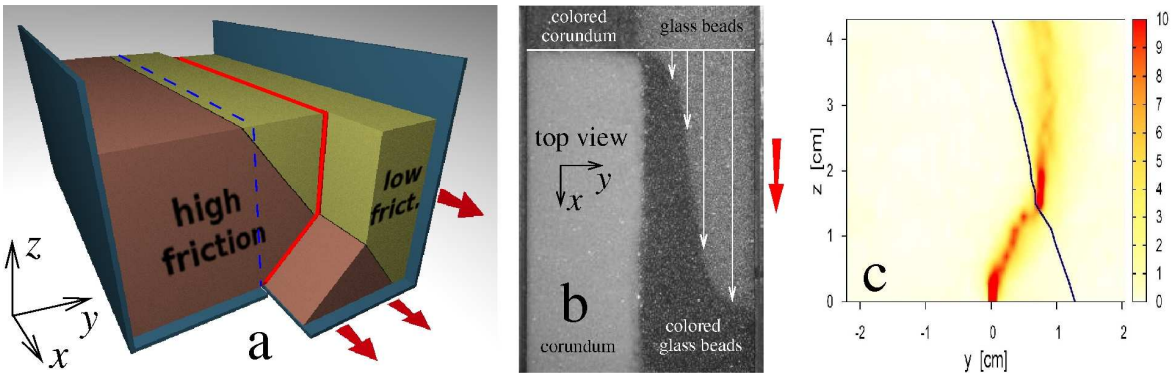

Fig. 2 *(a) Deformation of a granular material obtained by moving the L shaped boundary. In case of a homogeneous material the shear zone would be located in the middle of the cell as indicated by the dashed line. In a layered system however, the zone escapes the high friction part, changes direction at the layer boundary and comes to the top in the low friction part as it is indicated by the solid line. Deformation was visualized using colored samples as illustrated in panel (b). The experimentally reconstructed deformation profile (c) fully agrees with the expectation (a).*

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Grants and international cooperations

OTKA K 061075 Mesogens with polar ordering of non-chiral building blocks (Á. Buka, 2006-2010)

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[2] SK-12/2008 (Hungarian-Slovak bilateral) Magnetically active anisotropic fluids (N. Éber, 2009-2010)

NKTH TÉT AR-3/2008 (Hungarian-Argentinian bilateral) Transient and metastable states (Á. Buka, 2009-2011)

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-RAS (Hungarian-Russian bilateral) Boundary effects in complex systems (T. Tóth-Katona, 2008-2010)

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

— Prof. Antal Jákli: Liquid Crystal Institute, Kent State University, Kent, USA, June 21-July 21, 2010 (host: N. Éber)

— Andrew Konya: Kent State University, Kent, USA, June 03-July 10, 2010 (host: T. Börzsönyi)

— Prof. David Statman and Alex F. Erlwein: Allegheny College, Meadville, USA, June 21-July 30, 2010 (host: I. Jánossy)

— Anna L. Bitting: Allegheny College, Meadville, USA, June 21-July 30, 2010 (host: N. Éber)

— John P. Stenger: Allegheny College, Meadville, USA, June 21-July 30, 2010 (host: T. Börzsönyi)

— Marci L. Potuzko: Allegheny College, Meadville, USA, June 21-July 30, 2010 (host: T. Tóth-Katona)

Publications

Articles

F.1. Börzsönyi T, Unger* T, Szabó B; Shear zone refraction and deflection in layered granular materials; *Phys Rev E;* **80**, 060302(R)/1-4, 2009

F.2. Kumar* P, Heuer* J, Tóth-Katona T, Éber N, and Buka Á; Convection-roll instability in spite of a large stabilizing torque; *Phys Rev E;* **81**, 020702(R)/1-4, 2010

[2] National Office for Research and Technology Science and Technology

F.3. Salamon P, Éber N, Buka Á, Gleeson* JT, Sprunt* S, Jákli* A; Dielectric properties of mixtures of a bent-core and a calamitic liquid crystal; *Phys Rev E;* **81**, 031711/1-11, 2010

F.4. Éber N, Heuer* J, Stannarius* R, Tátrai* G, Buka Á; Director distortions and singularities in inhomogeneous fields; *Phys Rev E;* **81**, 051702/1-11, 2010

F.5. Obadović* DŽ, Vajda A, Jákli* A, Menyhárd* A, Kohout* M, Svoboda* J, Stojanović* M, Éber N, Galli* G, Fodor-Csorba K; Mesophase behaviour of binary mixtures of bell-shaped and calamitic compounds; *Liq Cryst;* **37**, 527-536, 2010

F.6. Kohout* M, Chambers* M, Vajda A, Galli* G, Domján* A, Svoboda* J, Bubnov* A, Jákli* A, Fodor-Csorba K; Properties of non-symmetric bent-core liquid crystals with variable flexible chain length; *Liq Cryst;* **37**, 537-545, 2010

F.7. Kopčansky* P, Tomašovičová* N, Koneracká* M, Timko* M, Závišová* V, Éber N, Fodor-Csorba K, Tóth-Katona T, Vajda A, Jadzyn* J, Beaugnon* E, Chaud* X; The structural instabilities in ferronematic based on liquid crystal with negative diamagnetic susceptibility anisotropy; *J Magn Magn Mat;* **322**, 3696-3700, 2010

F.8. Jánossy I; Kinetics of director gliding on a polymer – liquid-crystal interface; *Phys Rev E;* **81**, 031714/1-6, 2010

F.9. Mitróová* Z, Koneracká* M, Tomašovičová* N, Timko* M, Jadzyn* J, Vávra* I, Éber N, Fodor-Csorba K, Tóth-Katona T, Vajda A, Kopčansky* P; Structural transitions in nematic liquid crystals doped with magnetite functionalized single walled carbon nanotubes; *Phys Procedia*; **9**, 41-42, 2010

F.10. Kopčansky* P, Tomašovičová* N, Koneracká* M, Závišová* V, Timko* M, Tomčo* L, Éber N, Fodor-Csorba K, Tóth-Katona T, Vajda A, Jadzyn* J, Beaugnon* E, Chaud* X; Néel and Brownian rotation in ferronematics; *Phys Procedia*; **9**, 82-86, 2010

F.11. Kopčansky* P, Koval'chuk* A, Gornitska* O, Vovk* V, Koval'chuk* T, Tomašovičová* N, Koneracká* M, Timko* M, Závišová* V, Jadzyn* J, Éber N, Studenyak* I; Dielectric spectroscopy of liquid crystal doped with Fe_3O_4 nanoparticles; *Phys Procedia*; **9**, 36-40, 2010

F.12. 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*; accepted for publication

Conference proceeding

F.13. Obadović* DŽ, Stojanović* M, Cvetinov* M, Vajda A, Éber N, Lazar* D; The influence of x-ray radiation onto the phase transitions of some cholesteric liquid crystal mixtures; In: *Proceedings of the 10th International Conference on Fundamental and Applied Aspects of Physical Chemistry, September 21-24, 2010,* Belgrade, Serbia; Vol. II., pp. 423-425, 2010

G. RADIOFREQUENCY SPECTROSCOPY

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

Hydration of intrinsically disordered proteins. — Wide-line ^{1}H NMR signal intensity, spin-lattice and spin-spin relaxation rates and differential scanning calorimetry (DSC) measurements were done on avian (chicken and turkey) crystalline lenses between -70°C and -45°C to provide quantitative measures of protein hydration characteristics of the protein water interfacial region (Fig. 1). These measures are of paramount importance in understanding both the physiology of crystalline lens and its transitions to the cataractous pathological state characterized by the formation of opaque protein aggregates. Water mobility shows a characteristic transition at about -60°C, which is identified as the melting of the interfacial/hydrate water. The amount of water in the low-temperature mobile fraction is about h = 0.4 g water/g protein, which equals the hydration required for protein activity. The amount of mobile water is temperature-independent up to about -10°C, with a significant increase at higher temperatures below 0°C. Above 0°C, the relaxation processes can be described by a single (for spin-lattice relaxation) and by a triple (for spin-spin relaxation) exponential function. The spin-spin relaxation rate component of R_2 = 10-20 s^{-1} and its dynamical parameters characterize the interfacial water at ambient or physiological temperatures. When considered as an independent phase, the specific heat of the hydrate water obtained by a combination of DSC and NMR data in the temperature range -43°C to -28°C is higher than that of pure/bulk water. This discrepancy can only be resolved by assuming that the hydrate water is in strong thermodynamic coupling with the protein matrix. The specific heat for the system composed of the protein molecule and its hydration water is 4.6±0.3 J·g^{-1}·K^{-1}. Thus, in a thermodynamic sense, crystalline protein and its hydrate layer behave as a highly interconnected single phase.

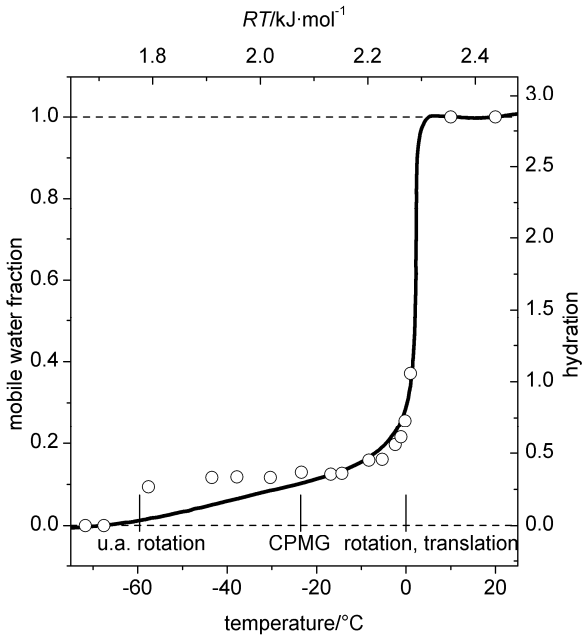

Fig. 1 *Mobile-water fraction measured by NMR and thermal analysis of the chicken eye lenses. Comparison of the liquid (mobile) water fraction calculated from the DSC curve (line) and the mobile ^{1}H (water) fraction measured by NMR (circles). The lowest temperatures where rotational (uniaxial or isotropic) or translational diffusion was detected are marked. The script CPMG refers to the lowest temperature where Carr-Purcell-Meiboom-Gill type echoes could be detected (that is the point where isotropic rotation starts).*

Parkinson's disease (PD) is a lingering neurodegenerative disease, which induces degeneration of substantia nigra in the brain typically above the age of 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. Besides wild-type protein,

[#] Ph.D. student

α-synuclein may also have several inherited, familial mutations related to PD, such as A53T, A30P, and E46K. α-synuclein is a small, highly soluble, heat-stable protein, which is expressed at high levels in the brain, where its normal function is not fully understood. α-synuclein belongs to the class of intrinsically disordered proteins. We have investigated the protein-solvent interfacial region by ^{1}H, ^{23}Na and ^{35}Cl NMR for wild-type and mutant α-synuclein variants. The hydrogen and the chlorine NMR signals show a concerted trend with changing temperature (Fig. 2). The sodium ions are embedded in a mobile neighborhood even at low temperatures where the hydrogen and chlorine nuclei can be considered as in a solid phase. The mobile surroundings of the sodium ions can be attributed to reorienting groups of the amino acid residuals. We have found marked differences in the amount and dynamic properties of the hydration for the α-synuclein variants. We relate these features to different tertiary structures and expect to find connections with the amyloid-forming propensities.

Metal-hydrogen systems. — We have investigated hydrogen charging (discharging) processes in $Pd_{0.90}Ag_{0.10}$-H alloys by simultaneous hydrogen concentration and nuclear spin-spin relaxation time measurements. We have found two-component spin-spin nuclear relaxation in the whole hydrogen concentration range. The results give the hydrogen quantity in both phases. The phases were identified as the α and the β phase, respectively, in the high concentration range. The two phases do exist even at the smallest detectable hydrogen content.

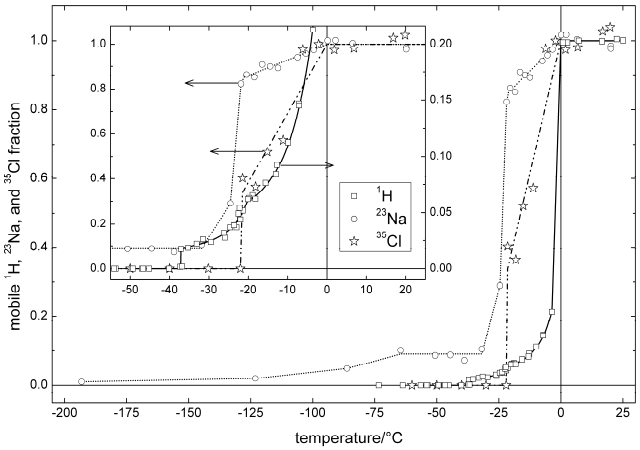

Fig. 2 *Temperature dependence of the mobile ^{1}H, ^{23}Na, and ^{35}Cl fraction measured by NMR for wild-type α-synuclein in Tris-buffer. The inset shows the temperature range at around the eutectic melting of the NaCl-H_2O system (-21°C).*

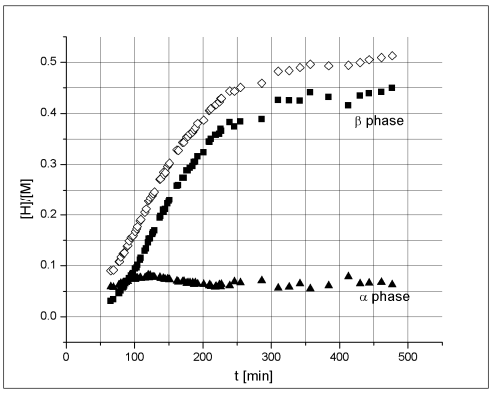

Fig. 3 *[H]/[M] values of $Pd_{0.90}Ag_{0.10}$-H obtained from CPMG T_2 measurements vs. duration of hydrogen exposure at 296 K. Triangles: [H]/[M] of α phase; circles: [H]/[M] of β phase; diamonds: sum of the two components.*

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Grants and international cooperations

OTKA K 62866	Collective dynamics of elastic lattices in disorder potential (F.I.B. Williams, 2006-2010)
SPEC – Saclay	Collaboration agreement with Service de Physique de L'Etat Condensé (SPEC) CEA-Saclay, France on electron crystals and nano-electronics (2005-2009)
OTKA NK 71582	Intrinsically disordered proteins: extension of the structure-function paradigm (project leader: P. Tompa, Institute of Enzymology, BRC, Hungarian Academy of Sciences; SZFKI participants: K. Tompa, M. Bokor; 2008-2010)

Publications

Articles

G.1 Tompa K, Bánki P, Bokor M, Kamasa P, Rácz* P, Tompa* P; Hydration water/interfacial water in crystalline lens; *Exp Eye Res;* **91**, 76-84, 2010

G.2 Vad* K, Hakl* J, Csik* A, Mészáros* S, Kis-Varga* M, Langer* GA, Pallinger Á, Bódog* M; Application of secondary neutral mass spectrometry in the investigation of doped perovskites; *Vacuum*; **84**, 144-146, 2010

Book chapter

G.3. Tompa K, Bokor M, Tompa* P; Chapter 12. Hydration of intrinsically disordered proteins from wide-line NMR; In: *Instrumental Analysis of Intrinsically Disordered Proteins: Assessing Structure and Conformation*.; Eds. Uversky V.N. and Longhi S. (Wiley, Hoboken, N.J.); pp. 345-368, 2010.

Other

G.4. Rácz* P, Bánki P, Bokor M, Kamasa P, Tompa* P, Tompa K; A szemlencse természettudományos szemmel (The eye lens viewed through the eye of a scientist, in Hungarian); Természet Világa; **141**, 439-442, 2010

H. ELECTRODEPOSITED NANOSTRUCTURES

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

Depth profile analysis of electrodeposited multilayers. — The previously developed sample preparation technique for reverse depth profile analysis was used in the study of Fe-Co-Ni alloys prepared with galvanostatic electrodeposition. This work was performed in collaboration with the Nuclear Research Institute of the HAS (Debrecen, Hungary). It was revealed that the deposition of the metal with the highest deposition preference (here, Fe) is deposited under mass transport controlled conditions. It was shown that the decay of the molar fraction of Fe in the initial zone of the deposit is in conformity with the semi-infinite planar diffusion model applied for the reactant (i.e., Fe^{2+} ion). The diffusion coefficients were also determined with conventional electrochemical methods like chronoamperometry or limiting current measurements on microelectrodes. For a low reactant concentration ($c(Fe^{2+})$ = 3 mmol/liter), the diffusion coefficients determined for the various methods are in excellent agreement. However, at higher reactant concentrations ($c(Fe^{2+})$ = 3–25 mmol/liter), the composition depth profile functions reveal that the diffusion of the reactant is abnormally fast, and the diffusion coefficients obtained are often by an order of magnitude larger than those determined with the conventional methods. Similar values can be found in studies concerning the electrochemical nucleation of metals on foreign substrates under diffusion control. These results indicate that the models with a normal diffusion process may not be applicable for modeling the ionic transport during electrodeposition.

Structure and giant magnetoresistance (GMR) of electrodeposited multilayers. — The influence of the current density applied during the deposition of the magnetic layers on the microstructure formation in electrodeposited Co-Cu/Cu multilayers and on their giant magnetoresistance (GMR) was investigated using a combination of magnetoresistance measurements and structural studies (carried out in collaboration with the Technical University Freiberg, Germany) such as wide-angle and small-angle X-ray scattering, high-resolution transmission electron microscopy, atomic force microscopy and chemical analysis. The magnetoresistance measurements revealed that a reduction of the current density stimulates a transition from the formation of the magnetic layers with predominantly ferromagnetic character to the formation of superparamagnetic regions. According to electrochemical considerations, such a change in the magnetic properties can be caused by an increased amount of Cu codeposited with Co at low current densities. It turned out from the structural studies that at low current densities actually a pronounced segregation of Co and Cu occurs. In accordance with their very low mutual solubility at room temperature, no atomic scale intermixing of Co and Cu could be detected. The segregation of Cu and Co was related to the fragmentation of the magnetic layers, to the enhancement of the local lattice strains, to the increase of the interface corrugations, to the partial loss of the multilayer periodicity and finally to the formation of Co precipitates in the Cu matrix.

Modelling the field dependence of magnetoresistance of GMR multilayers with various couplings and anisotropies. — In order to better understand the role of possible couplings in determining the giant magnetoresistance (GMR) behaviour of multilayers, a knowledge of the dependence of the *GMR* on magnetic field *H* appears to be useful. Since a few specific cases have only been treated theoretically in the literature, it was decided to

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carry out a modeling of the *GMR*(*H*) curves of ferromagnetic/non-magnetic (FM/NM) multilayers with various interlayer couplings and anisotropies. For simplicity, we focused on a trilayer structure ($FM_1/NM/FM_2$) corresponding fairly well to the case of a large number of FM/NM bilayers. To carry out the calculations, some fundamental assumptions were made: (i) each FM layer consists of a single domain and the magnetizations are in the layer planes; (ii) the magnetization of each layer is the same; (iii) the magnetization vectors rotate in the plane of the layers in an external magnetic field. In order to calculate the *GMR*(*H*) function, we need to know the magnetization process in the trilayer, i.e., the *M*(*H*) function. Therefore, first we calculate the equilibrium angle $\varphi(H)$ between the two magnetization vectors as a function of the field by minimizing the total energy of the multilayer. Since the dependence of the *GMR* on φ was theoretically calculated by Blaas et al. [*Eur. Phys. J. B* **9**, 245 (1999)], thus we can get the *GMR*(*H*) function. Along this line, the *M*(*H*) and *GMR*(*H*) curves were calculated for several specific cases: (i) AF coupling; (ii) orthogonal coupling; (iii) AF coupling and orthogonal coupling; (iv) AF coupling and uniaxial anisotropy with *H* along the easy axis; (v) AF coupling and uniaxial anisotropy with *H* along the hard axis; (vi) orthogonal coupling and uniaxial anisotropy with *H* along the easy axis. Most of these configurations have not yet been treated formerly; in cases for which results were reported in the literature for *M*(*H*) and *GMR*(*H*), our results agree with those reported previously.

Nanoscale phase separation - Rate and mechanism of symplectite formation. — Symplectites are vermicular intergrowth of two or more mineral phases showing high degree of spatial organization. Products of mineral reactions in metamorphic rocks frequently form the same microstructure, even though phases of the symplectites and the symplectite forming reactions are different. We study the general controls of symplectite formation through the example of garnet breakdown in lower crustal garnet granulite xenoliths from the Bakony–Balaton Highland Volcanic Field, Central Pannonian Basin, Hungary. The reaction includes the replacement of a homogeneous precursor phase along a moving interphase boundary by a symplectite of three nanometer-sized phases forming vermicular intergrowths. The TEM study of ultrathin foils prepared from the reaction products parallel with and perpendicular to the reaction interface by focused ion beam (FIB) technique has shown that the redistribution of material during phase separation takes place by fast diffusion in a few nanometer-wide zone right at the reaction front parallel to the interphase boundary. The rate at which the reaction front propagated into the precursor garnet was studied by applying irreversible thermodynamics. The suggested thermodynamic model provides constraints on the interplay of component diffusion in the migrating reaction front and the formation of new phase contacts in symplectites.

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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, micostructure 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)

Long-term visitor

— M. Jafari Fesharaki, Ph.D. student, Arak University, Iran, Feb. – July 2010, (hosts: L. Péter and I. Bakonyi)

Publications

Articles

H.1. Bakonyi I, Péter L; Electrodeposited multilayer films with giant magnetoresistance (GMR): progress and problems; *Progr Mater Sci.;* **55**, 107-245, 2010

H.2. Csik* A, Vad* K, Langer* GA, Katona* GL, Tóth-Kádár E, Péter L; Analysis of Co/Cu multilayers by SNMS reverse depth profiling; *Vacuum;* **84**, 141-143, 2010

H.3. Dégi J, Abart* R, Török* K, Bali* E, Wirth* R, Rhede* D; Symplectite formation during decompression induced garnet breakdown in lower crustal mafic granulite xenoliths: mechanisms and rates; *Contrib Mineral Petrol;* **159**, 293-314, 2010

H.4. Péter L, Csik* A, Vad* K, Tóth-Kádár E, Molnár* G; On the composition depth profile of electrodeposited Fe-Co-Ni alloys; *Electrochim Acta;* **55**, 4734-4741, 2010

H.5. Tóth BG, Péter L, Révész* Á, Pádár J, Bakonyi I; Composition and temperature dependence of the electrical resistivity and the anisotropic magnetoresistance (AMR) of electrodeposited Ni-Co alloys; *Eur Phys J B;* **75**, 167-177, 2010

H.6. 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;* accepted for publication

Book chapter

H.7. Péter L, Bakonyi I; In: *Nanomagnetism and Spintronics: Fabrication, Materials and Characterization, and Applications*; Eds.: Nasirpouri F and Nogaret A, World Scientific, Singapore; Ch. 5, pp. 89-120, 2010

Others

H.8. Péter L; A mítosz varázsa (Fascination of the Myth, in Hungarian); *Magyar Tudomány* **171**, 95-97, 2010

See also: D.6., I.8.

I. METALLURGY AND MAGNETISM

L.K. Varga, É. Fazakas[#], P. Kamasa

Metallurgy. — An electronic rule was found for the hardness and thermal stability of Al based amorphous alloys: both parameters increase with the average valence electron number (see Fig. 1). Complementing our experimental results obtained for Al-based amorphous alloys with the literature data for other conventional and bulk amorphous alloys, we have found a maximum strength and thermal stability corresponding to e/a ~ 6-6.5 (see Fig. 2).

As to the application of amorphous alloys, surface coatings were prepared with an oxy-acetylene thermal spray coating device from Castolin (DS8000 with an SSM40 modulus) whereby a Cu-Ti-Zr alloy was deposited onto copper surface and $Al_{88}Mm_5Ni_5Fe_2$ and $Al_{85}Mm_8Ni_5Co_2$ gas-atomized powders onto Al-Si substrate. The screened powder (D <200 μm) was deposited onto a roughened target resulting in a coating with an average thickness of 150-200 μm. The typical temperature near the exit nozzle in this setup is well above the melting point of the individual powder particles. The cooling rate was not high enough to form an amorphous structure for the coating droplet, nevertheless, the good glass-former compositions yielded a nanosized grain structure in both cases. For the Cu-Ti-Zr coating, a tendency to solid-state amorphization could be observed after surface mechanical attrition treatment. The coatings presented high hardness, good wear behavior and corrosion resistance.

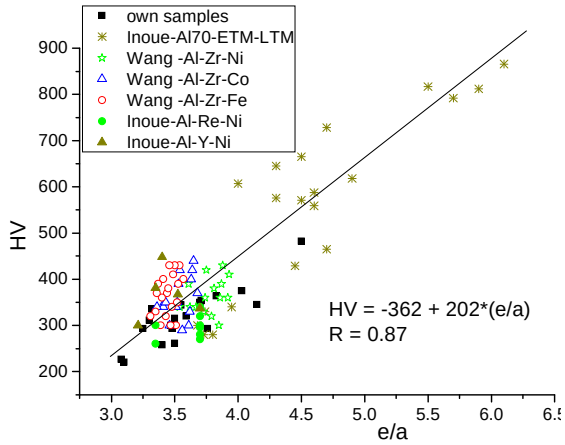

Fig. 1 *Vickers hardness for Al-based amorphous alloys as a function of the total valence electron number(e/a).*

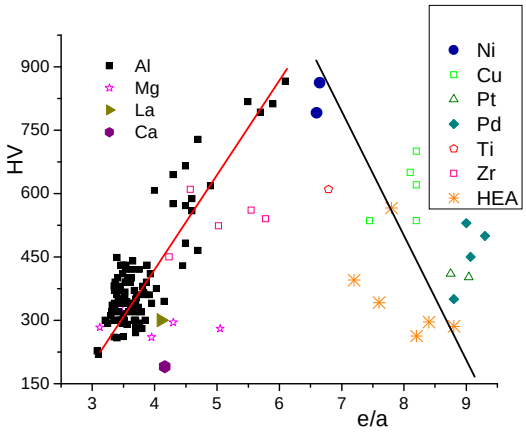

Fig. 2 *Comparison of the hardness behavior of conventional and bulk amorphous alloys based on the elements indicated in the inset.*
Some data for single-phase high-entropy alloys (HEA) are also indicated.

Soft magnetic nanocrystalline alloys. — A model of Steinmetz's approximation, based on the hyperbolic model, was developed. The Steinmetz's law states that the hysteresis loss (W) depends on the height of the minor loop (B_m) as $W = K \cdot B_m^p$ where *K* is a material constant and *p*, the exponent for soft ferrous materials, falls between 1.6 and 2, based on practical experience. The model has been applied for NO Fe-Si electrotechnic steels and ferrites.

A test bank was designed and built for our industrial partners in order to check the electromagnetic interference (EMI) filters in industrial environments. In these EMI filters,

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the inductive cores prepared from Finemet type nanocrystalline alloy ribbons will be tested after different experimental heat treatments.

Calorimeter for *in-situ* monitoring polymerization reaction in vacuum deposition chamber. – The DSC probe-head for *in situ* investigation of polymerization process in the vacuum deposition chamber was developed in the frame of the Hungarian-Russian Academic Exchange Program. The probe-head is designed as a heat-flux type calorimeter (Fig. 3, left).

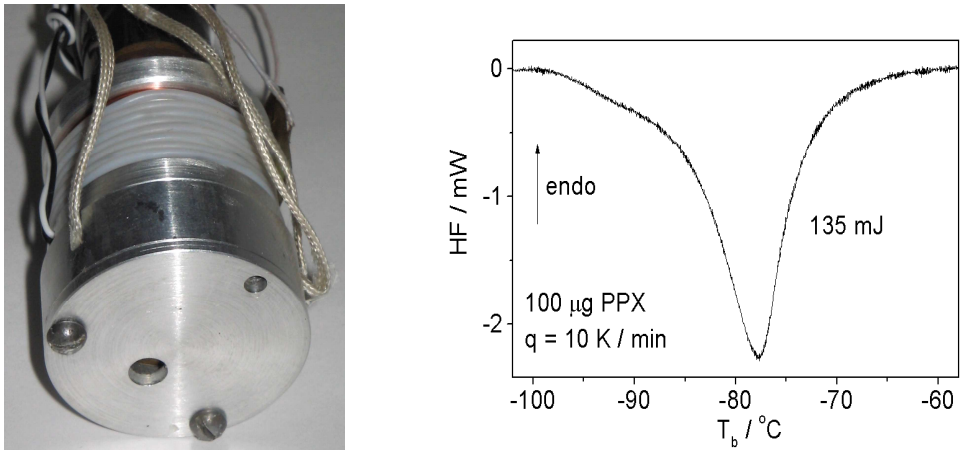

Fig. 3 *The calorimetric cell construction (left) and heat flow recorded during polymerization of poly(para-xylylene) (PPX) immediately after deposition during heating program in vacuum chamber (right).*

The polymerization mostly takes place at low temperatures and *in-situ* thermal analysis requires a technique which allows to carry out the experiment in one place. By placing the calorimetric unit in the deposition vacuum chamber, it is possible to carry out polymerization with simultaneous recording of the thermal effect during all processes. It is possible to obtain certain thickness of the film at exactly controlled mode of deposition and polymerization: substrate temperature, annealing temperature and heating temperature profile. Heating rate is available from isothermal annealing up to 80K/min linear scan in the range between LN_2 temperature and +200°C. Sensitivity of the probe-head of 50 μW is sufficient to measure reactions taking place in a few microgram sample.

As an example of the utilization of the new instrumentation, the right panel of Fig. 3 shows the result obtained for the solid-state polymerization of poly(para-xylylene) immediately after deposition in vacuum chamber.

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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, 2008-2010)

HAS-PAS Hungarian-Polish Academy Exchange Programme: Investigation of thermo-physical properties of coatings (P. Kamasa, 2008-2010)

HAS-RAS Hungarian-Russian Academy Exchange Programme: Calorimetric study of phase transformations (P. Kamasa, 2008-2010)

TOMMY-INVEST ELECTRONICS LTD. Testing, designing and producing inductive cores for the inductive electronic component market (Project leader: L.K. Varga, 2010)

Publications

Articles

I.1. Fazakas É, Varga* B, Varga LK; Bulk amorphous and nanocrystalline aluminium based alloys obtained by hot pressure consolidation; *J Optoel Adv Mater – Symposia*; **1**, 983-985, 2009

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I.3. Henits* P, Révész* Á, Schafler* E, Szabó* PJ, Lábár* JL, Varga LK, Kovács* Zs; Correlation between microstructural evolution during high-pressure torsion and isothermal heat treatment of amorphous $Al_{85}Gd_8Ni_5Co_2$ alloy; *J Mater Res;* **25**, 1388-1397, 2010

I.4. Henits* P, Kovács* Zs, Schafler* E, Lábár* JL, Varga LK, Révész* Á; Nanocrystallization in $Al_{85}Ce_8Ni_5Co_2$ amorphous alloy obtained by different strain rate during high pressure torsion; *J All Comp;* **504S**, S91-S94, 2010

I.5. Hóbor* S, Kovács* Zs, Zhilyaev* AP, Varga LK, Szabó* PJ, Révész* Á; High pressure torsion of Cu-based metallic glasses; *J Phys: Conf Series;* **240**, 012153/1-4, 2010

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I.8. Ristić* R, Babić* E, Pajić* D, Zadro* K, Kuršumović A, Figueroa* IA, Davies* HA, Todd* I, Varga LK, Bakonyi I; Properties and atomic structure of amorphous early transition metals; *J All Comp;* **504S**, S194-S197, 2010

I.9. Srivastava* SK, Srivastava* VK, Joshi* A, Kamasa P, Varga LK, Khovaylo* VV, Chatterjee* R; A low temperature anomaly observed in off-stoichiometric Ni-Mn-Ga system studied by higher harmonic ac-susceptibility measurements; *App Phys Lett;* **97**, 122505/1-3, 2010

I.10. Takács* J, Kovács* Gy, Varga LK; Modeling the Steinmetz's law for soft steel; *Eur Phys J Appl Phys;* 51**,** 20801/1-3, 2010

I.11. Varga* B, Fazakas É, Varga LK; Dilatometer study of aluminium-silicon based alloys with metastable structures; *Materials Science Forum*; **649**, 529-532, 2010

I.12. Henits* P, Révész* Á, Varga LK, Kovács* Zs; The evolution of the microstructure in amorphous $Al_{85}Ce_8Ni_5Co2$ alloy during heat treatment and severe plastic deformation: A comparative study; *Intermetallics;* accepted for publication; DOI: 10.1016/j.intermet.2010.10.007

I.13. Révész* Á, Szommer* P, Szabó* PJ, Varga LK; Microstructure and morphology of Cu-Zr-Ti coatings produced by thermal spray and treated by surface mechanical attrition; *J All Comp;* accepted for publication; DOI: 10.1016/j.jallcom.2010.10.170

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I.15. Gautam* S, Kane* SN, Kim* JY, Varga LK, Song* JH, Chae* KH; XAS and XMCD studies of amorphous FeCo ribbons; *J Non-cryst Solids*; accepted for publication

Conference proceedings

I.16. Stojanova* L, Fazakas É, Varga LK, Yankova* S, Russew* K; Thermal stability and viscosity of rapidly solidified amorphous alloys $Al_{85}Ni_5Co_2RE_8$ (RE= Gd, Ce, U) (in Bulgarian); In: *Proc. 25th Natl. Conf. on Non-Destructive Testing*; Nauchno Izvestiya na HTCM (Bulgaria) ISSN 1310-3946; **27,** 179-185, 2010

See also: D.6., G.1., G.4.

J. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

L. Rosta, L. Almásy, L. Cser, J. Füzi, Gy. Káli, Z. László, A. Len, M. Markó[#], A. Meiszterics[#], F. Mezei, G. Nagy[#], J. Orbán[#], Zs. Sánta, A. Szakál[#], N.K. Székely[#], Gy. Török, R. Ünnep[#], T. Veres

Neutron scattering equipment. — In 2010, the 10 MW Budapest Research Rector (BRR) with its experimental facilities on the KFKI campus has been awarded the title of "Strategic Research Infrastructure" within the national infrastructure Roadmap. Indeed, it is a unique large-scale facility in the Central European region, a basis for domestic and international user community to serves for exploratory and applied research as well as for methodical developments. We operate a number of neutron scattering instruments (small angle scattering spectrometer, diffractometer, reflectometer, three-axis spectrometers). These devices require a constant technical modernisation and upgrade. One of the key issues for the improvement of the spectrometer performance is the neutron beam delivery system or in other words the neutron guides. A new feature of neutron guides has been studied and completed this year.

Neutron supermirrors were discovered by F. Mezei in 1976 in Budapest; then since the application of magnetron sputtering techniques for the large scale productions of supermirrors (SM) in the middle of nineties, the construction of SM guides in neutrons centres has become a $ multimillion venture. Due to multiple reflections in neutron guides, the reflectivity decrease of neutron supermirrors deserves careful examination. One possible cause of reflectivity loss is the contamination by hydrogen-containing compounds (large incoherent scattering cross section), from vacuum pumps and the atmosphere. In our experiments vacuum pump oil was deposited on the surfaces of supermirror samples and the average film thickness was measured by weighing before and after deposition, also locally by optical interference. Inhomogeneities and drop formation were observed by optical microscope. The reflectivities of clean and oil-covered supermirrors were measured at the constant wavelength (λ=4.2 Å) reflectometer of the Budapest Research Reactor.

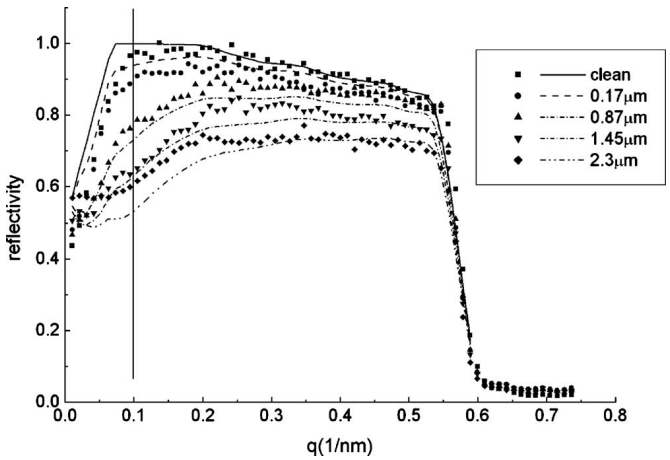

Fig. 1 *Measured (line) and calculated (dots) reflectivity of the supermirrors covered by oil of various thickness. (Left of the perpendicular line the reflectivity is distorted by geometrical effects.)*

We calculated the reflectivity applying the Parratt method. On Fig. 1 we can see the comparison of the measured and calculated reflectivities (the finite sample and slit sizes were considered). The drop formation can not be taken exactly into account; there is some deviation between calculated and measured values for the thickest oil films. Monte Carlo simulations predict exponential decreasing of neutron yield as a function of the oil

[#] Ph.D. student

thickness. The shape of the beam is also distorted in the model calculation, this effect could be used to diagnose the presence of contamination using the pin-hole method.

SANS study of solvent effect on the structure of epoxy gels. — A series of hydrophilic epoxy networks was prepared by end-linking reaction of *α,ω*-diamino terminated poly(oxypropylene)-block-poly(oxyethylene)-block-poly(oxypropylene) (POP-POE-POP) of molar mass 600 g.mol^{-1}, and diglycidyl ether of Bisphenol A propoxylate (PDGEBA) at various initial ratio of reactive groups $r=2[NH_2]_0/[E]_0$. The networks prepared were swollen to equilibrium in deuterated methanol (CD_3OD) and heavy water (D_2O), respectively. Whereas methanol is good solvent for all the blocks built into the network (POE, POP and PDGEBA), water is good solvent for POE only. Consequently, SANS patterns of the gels obtained by swelling of networks in CD_3OD and D_2O differ significantly as illustrated in Fig. 2. In networks swollen in methanol (Fig. 2a), the scattering is governed by frozen and dynamic inhomogeneities, respectively, due to network connectivity and thermal movement of polymer segments. Unlike this, in networks swollen in water (Fig. 2b), above contributions to SANS are superimposed by inhomogeneities due to nanophase separation of the system into water-rich and water-poor domains. The domains exhibit a locally lamellar order as proved by successful fitting of SANS patterns to the Teubner-Strey model.

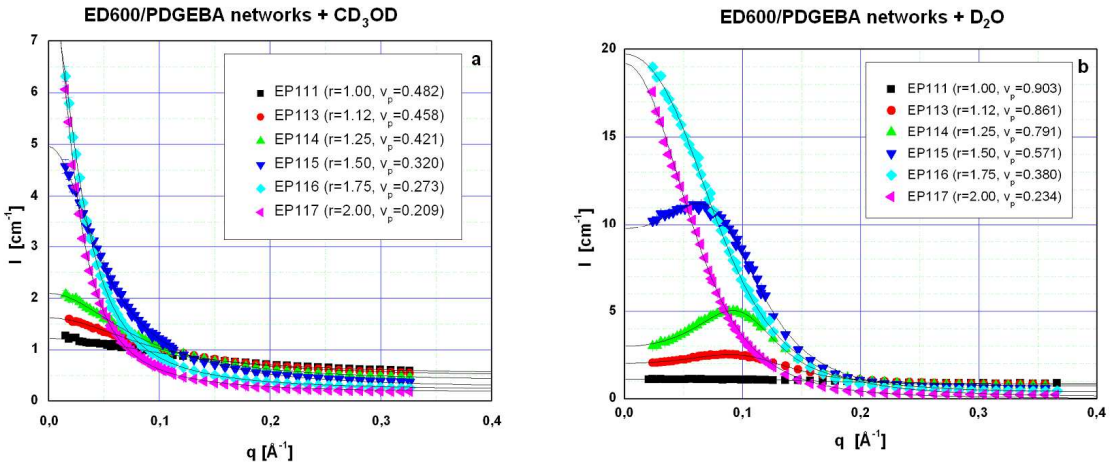

Fig. 2 SANS scattering profiles obtained from the epoxy networks swollen to equilibrium in CD_3OD (a) and D_2O (b) at 25 °C. Solid lines represent fits according to model developed for polymer networks swollen in good solvent (a) and Teubner-Strey model (b). v_p denotes the polymer volume fraction in gels.

Cultural heritage. — Since last year we take part in a large EU FP7 project named CHARISMA, to provide analytical scientific approach and instrumentation for the investigation of ancient objects. In this regard a preliminary study of medieval swords by time-of-flight neutron powder diffraction (TOF-NPD) was performed at BRR. The aim of the experiment was to present the applicability of the method and the instrument itself for non-invasive characterization of archeological artifacts made of carbon steel. The following characteristics were planed to determine: phase composition (for steel phases as ferrite, cementite, as far as possible martensite and non-steel phases), degree of alloying of the main phase, total carbon content, texture and the average internal stress and dislocation density. Four medieval – or believed to be that – swords have been studied. **Sword1**

strongly corroded but together with **Sword2** were visibly Damascus blades, certificated archeological objects. **Sword3** and **Sword4** were in good state but not certificated. Based in our experiments we assumed the following, concerning the texture: although the anisotropy in hot worked metal is much weaker than in a cold worked one, we have found that it is extremely low in the investigated objects thanks to the good manufacturing. On the other hand, the nature of the data seems to be typical for different style blades. In phase analysis: all the blades show high, but different cementite concentration, but no other phase has been found in the applied scattering vector range. Concerning the alloying degree of the main ferrite phase, the peak shift carries information rather on the final heat treatments, while the amount of the carbon in the ferrite depends mainly on the cooling rate.

	Broadening [Å] (±0.00006Å)	Relative peak shift (±0.00005)	Cementite content[wt%] (±3)	Carbon content in ferrite [at.%] (±0.00003)
Sword1	0.00075	0.00059	13.1	0.0028
Sword2	0.00015	0.00011	16.0	0.0005
Sword3	0.00064	0.00031	17.8	0.0014
Sword4	0.00000	0.00041	8.76	0.0019

Table 1. *The main parameters gained from the diffraction patterns.*

To obtain information on stress and strains the peak shape analysis of the high resolution spectra were used. It was clearly visible, that the peak profiles show Lorentzian broadening compared to pure iron. These values – i.e. the broadening compared to pure iron – are presented in Table 1. It is interesting to note that ***one*** of the swords shows no line broadening. More accurate results can be gained using a correct model for the inelastic scattering part (Fig. 3), which is a completely new approach in this kind of studies.

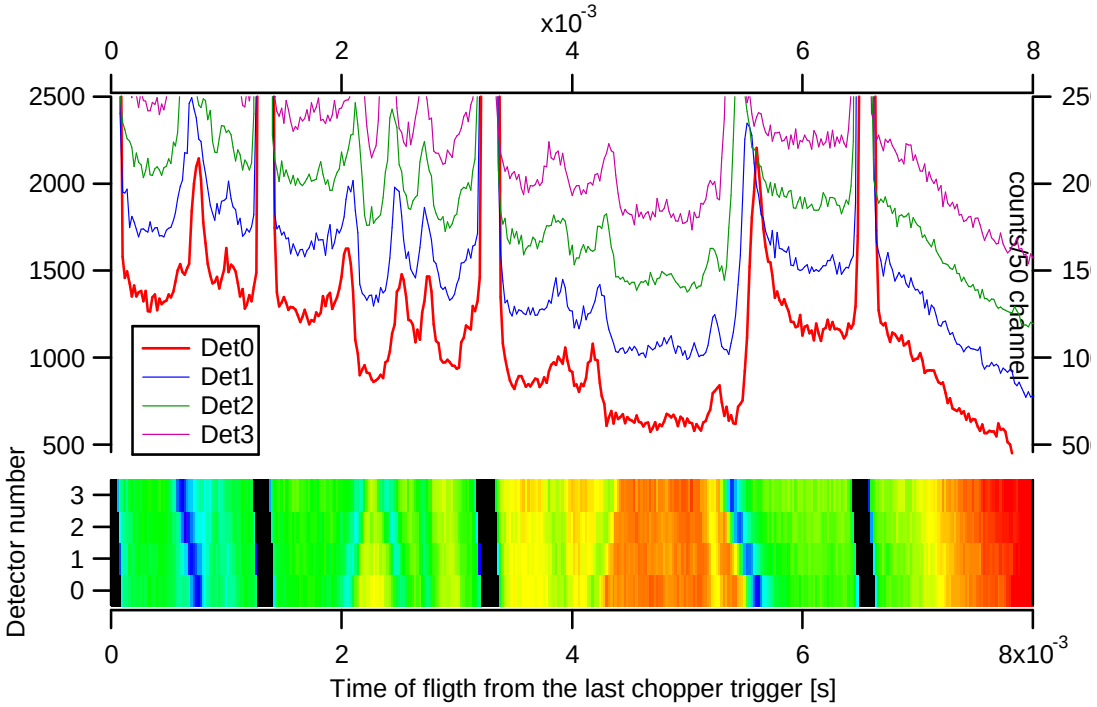

Fig. 3 *The angular behavior of the inelastic part of the spectra. While weak elastic peaks are parallel to the other stronger peaks (black region) the inelastic ones are inclined depending either annihilation or emission.*

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Grants and international cooperations

EU-FP7-CP-CSA-INFRA-2008-1.1.1 Number 226507-NMI3 – Integrated Infrastructure Initiatíve 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)

OMA 75öu2 Bilateral Austro-Hungarian Cooperation, Experimental determination of local lattice distortions in binary systems using neutron scattering (L. Cser 2009-2010)

Long-term visitors

— G. Peppy, Laboratoire Léon Brillouin (LLB), CEA Saclay, France, February 7-17, May 24 – June 3 and September 15 – 24, 2010 (host: L. Rosta)

— M. Avdeev – Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research Dubna, Russia, August 5 –September 5, 2010 (host: L. Rosta)

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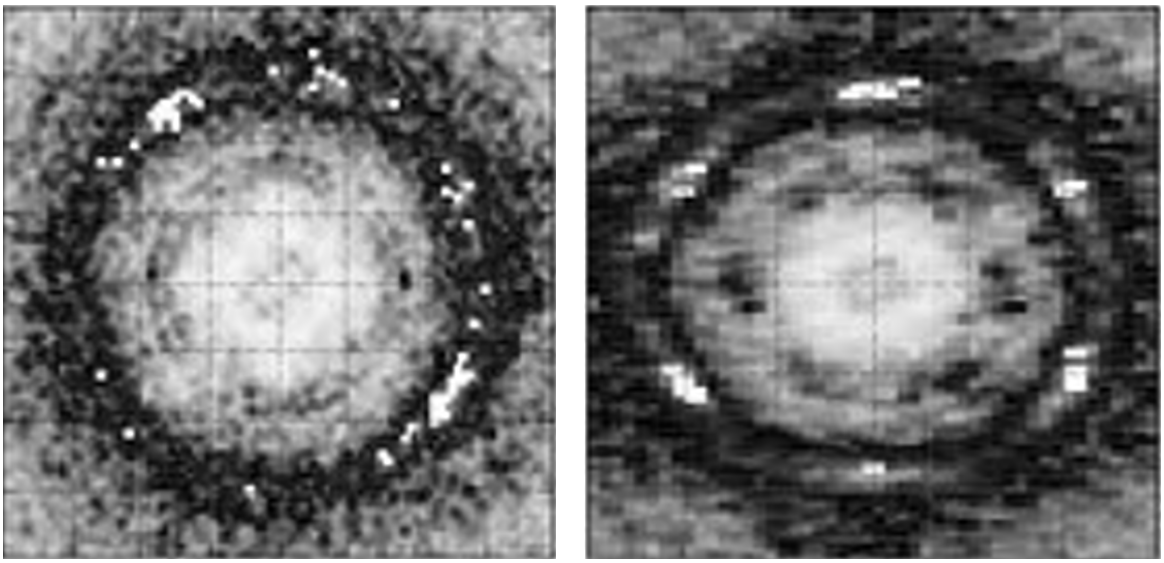
K. NEUTRON SCATTERING

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

Plastic crystals. — *Carbon tetrabromide*, CBr_4, is one of the molecular systems that can form plastic crystalline phases in which molecular centers (here: C atoms) possess long range crystalline order whereas ligands (here: Br atoms) do not, since molecules can rotate nearly freely. The total scattering structure factors of the ordered and plastic crystalline and liquid phases of CBr_4 have been measured by neutron powder diffraction. For the crystalline phases, Bragg and diffuse scattering could be separated and interpreted by the RMCPOW Reverse Monte Carlo (RMC) algorithm. From the particle configurations that were consistent with the measured total scattering powder patterns, the single crystalline scattering patterns could be calculated (see Fig. 1) and compared to literature data.



a) b)

Fig. 1 *a) Calculated X-ray single crystal diffraction pattern of the plastic phase of carbon tetrabromide projected along the [001] direction. b) Same as a) but along the [111] direction.*

From detailed analyses of partial radial distribution functions, orientational correlation functions and condensed views of the Bravais cells of the crystalline phases it was concluded that the essence of the order-disorder transition in this (and similar tetrahedral) system(s) is the appearance of the 2:2 orientations (in terms of Rey's classification) for neighboring molecules.

Lead based rare earth perovskites. — Perovskites $La_{1-y}Pb_yMnO_3$ ($y \leq 0.5$) are ferromagnets with Curie temperature T_C increasing linearly with x to 355 K for x=0.5 and display colossal magnetoresistance (CMR) effects. Doping of the Mn sites with Fe dramatically alters material properties leading to a wide scope of applications of $La_yPb_{1-y}Fe_{1-x}Mn_xO_3$ such as catalysts, electrode materials in solid oxide fuel cells, exhaust gas sensors, membranes for separation processes etc. We have investigated and analysed the structure by X-ray diffraction (XRD) and neutron diffraction (ND).

Simultaneous XRD and ND Rietveld analyses showed that $La_{0.5}Pb_{0.5}FeO_3$ (x=0) is best described in orthorhombic Pnma space group, similarly to $LaFeO_3$. The remaining crystal structures have Imma symmetry (except R-3c for x=1). Though Mn^{3+} and Fe^{3+} are with

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practically identical ionic radii (0.645 Å), doping affects the crystal structure: there are sizeable lattice deformations reflected by changes in unit cell volume, bond angles and cation-oxygen distances. Magnetic interactions are strongly affected: the Mn rich compounds (x > 0.5) display ferromagnetism whereas those with high Fe content are canted antiferromagnets. The magnetic structure of x=0 is of G_xF_z-type with main component of the effective magnetic moment on the iron site S_x = 3.6± 0.2 μ_B.

Borosilicate glasses. — Multi-component alkali borosilicate glasses are known as most promising host materials for immobilizing high-level radioactive wastes, like U-, Pu-, Th-oxides. We have successfully prepared $(65\text{-}x)SiO_2 \cdot xB_2O_3 \cdot 25Na_2O \cdot 5BaO \cdot 5ZrO_2$ (x=5-20 mol%) matrix glasses and the same compositions loaded with 30 wt% UO_3. Both systems have been investigated by neutron diffraction and high energy X-ray diffraction. The short range atomic structure has been analysed by direct Fourier-transformation method and RMC modelling. The basic network was found to consist of tetrahedral SiO_4 units and tetrahedral BO_4 and trigonal BO_3 units (Fig. 2). From the characteristic features of the uranium surrounding revealed from the U-O first neighbour atomic correlation, and from the second neighbour U-Si, U-B, U-Na and U-Zr correlations we have concluded that uranium ions take part in the network forming, which may be the reason for the observed good glass stability and hydrolytic properties.

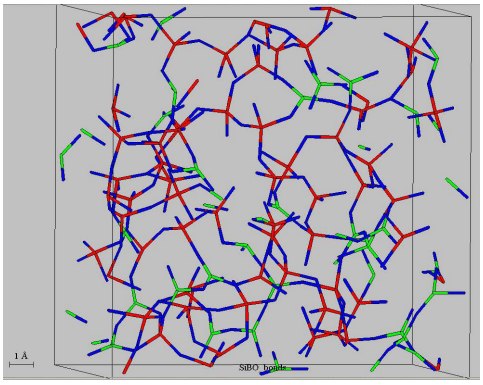

Fig. 2 *Schematic representation of the basic network structure of borosilicate glass, with 10 mol% B_2O_3: Si (dark grey), B (light grey) and O (grey) bond lines*

Chalcogenide glasses. — Glasses suitable for applications in the far IR range can be obtained by alloying Te-rich Ge-Te glasses with a third component (Ga, Se or I). The structure of bulk glass formers $Te_{78}Ge_{11}Ga_{11}$, $Te_{70}Ge_{20}Se_{10}$ and $Te_{73}Ge_{20}I_7$ (denoted with TGG, TGS and TGI, respectively) was investigated by neutron and X-ray diffraction measurements as well as extended X-ray absorption spectroscopy (EXAFS) experiments at Ga, Ge, Se, Te and I K-absorption edges. For each composition, the experimental datasets were fitted by the RMC simulation technique. N_{Te}, the average coordination number is close to 2 in TGI, TGS as well as in binary $Te_{85}Ge_{15}$ while it is as high as 2.39±0.2 in TGG. It was also observed that in TGG $N_{TeGe}+N_{TeTe}$ is very close to 2 suggesting that Ga participates in the ‘third bond‘ of Te atoms. Thus, unlike Se or I, Ga does not build into the Ge-Te covalent network. Instead, it forms a bond with the non bonding p electrons of Te, which results in an increase of the average Te coordination number. This is consistent with the expected role of Ga in the initial composition: catching the Te lone electron pairs to prevent tellurium from crystallizing. Fig. 3 shows a schematic model of TGG based upon the above results.

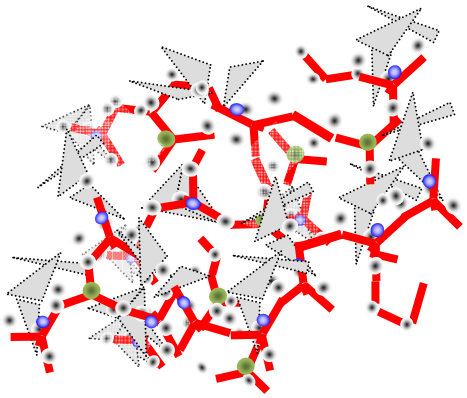

Fig. 3 *A model structure of $Te_{78}Ge_{11}Ga_{11}$ with threefold coordinated Te atoms, showing (by the thick dark grey line) the covalent network defined by Ga, Ge and Te atoms*

Bond lengths also clearly show that the third component has strong influence on the average Te-Te distance. While the Ge-Te distance is essentially the same in all alloys investigated

(2.60±0.02 Å), the Te-Te bond is significantly longer in TGG (2.80±0.02 Å) than either in TGS (2.73±0.02 Å) or in TGI (2.70±0.02 Å). The Te-Te distance in $Te_{85}Ge_{15}$ (2.75±0.02 Å) is just half way between the corresponding values of TGI and TGG. Our results suggest that the poor glass forming ability of Ge-Te alloys is improved by entirely different strategies. While I and Se build in the covalent network making Te-Te bonding stronger, Ga increases the average coordination number of Te (and also network connectivity) but decreases Te-Te bond strength.

Liquids. — Neutron and X-ray weighted total scattering structure factors of *liquid methyline halides* (methylene-chloride, -bromide and –iodide, CH_2Cl_2, CH_2Br_2 and CH_2I_2) have been measured and interpreted by means of RMC modeling. For each material the two sets of diffraction data were modeled simultaneously, thus providing sets of particle coordinates which were consistent with two experimental structure factors within errors. From these particle configurations, partial radial distribution functions (PRDF), as well as correlation functions characterizing mutual orientations of molecules as a function of distance between molecular centers were calculated. Concerning these latter, the concept of Rey has been extended to molecules with two types of ligand (here: H atoms and Cl, Br or I atoms). It was shown that the neighboring molecules most frequently turn towards each other by one of their H-X 'edges' (X: Cl, Br or I). It has become apparent that the structure of liquid methylene chloride is substantially different from that of the two close relatives: it exhibits stronger orientational ordering, icluding better recognisable dipole-dipole correlations.

A detailed study of the microscopic structure of an electrolyte solution, *cesium bromide (CsBr) in water*, was carried out. For revealing the influence of salt concentration on the structure, CsBr solutions at concentrations of 0.9, 4.5 and 7.6 molar % were investigated. For each concentration, we combined total scattering structure factors from neutron and X-ray diffraction and 10 partial PRDFs from molecular dynamics simulations in one single structural model, generated by RMC modeling. We were able to show that for cesium bromide solutions the level of consistency between simulations that use simple pair potentials and experimental structure factors is nearly quantitative up to a salt concentration of about 4.5 molar %. Most of the inconsistencies seem to be caused by water-water distribution functions. It was found that the average angle of Br…H-O particle arrangements, characteristic to anion-water hydrogen bonds, is closer to 180^o than that found for O…H-O arrangements (water-water hydrogen bonds), even though not every water molecule around an anion is H-bonded to the anion.

Reverse Monte Carlo modeling of small angle scattering (SAS) experimental data – A new software code, RMCSANS, has been developed which is able to model the inter-particle structure in the nanometer to micrometer range via using small angle neutron and X-ray scattering data. The software was thoroughly tested using quasi-experimental data with known structure. The most substantial finding originating to this testing phase was that although 'measured' SAS intensities could be reproduced quantitatively, the range of structures consistent with an experimental *I(Q)* is very wide. That is, SAS *I(Q)*'s in general are information poor and therefore, it is advisable to combine SANS/SAXS results with further experimental evidence.

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Grants and international cooperations

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)

EU-FP7 N226507-NMI3 Access to Research Infrastructures: neutron diffraction (E. Sváb, 2009-2010)

TéT UA-32/2008 (Hungarian-Ukrainian bilateral) Structural study of environmentally 'green' glassy semiconductors for optoelectronic application (P. Jóvári, 2009-2010)

IAEA MOR4018/01/01 (International Atomic Energy Agency) Use of the Lateral Channels of the Triga Mark II Research Reactor, Phase III, Centre d'Etudes Nucléaires de la Maâmoa, Morocco (L. Kőszegi, 2010)

Long-term visitors

— A. Vrhovšek, University of Ljubljana (1 March – 31 May 2010; host: L. Pusztai)

Publications

Articles

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See also: I.6.

L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, P. Dombi, N. Kroó, M. Lenner, P. Rácz, S. Varró

Experimental research. — We investigated photoemission and electron acceleration phemonena in surface plasmon fields induced by few-cycle laser pulses with various laser sources. We could demonstrate that high-energy electrons in the keV range can be generated even in this extreme parameter regime (when the electrons spend only a few optical cycles in the accelerating field), moreover, we demonstrated strong-field photoemission with extremely low focused laser intensities. This was possible utilizing the field enhancement of surface plasmons with respect to the field of the plasmon inducing laser light. By achieving field enhancement factors of $> 20\times$, we could induce strong-field transition at ~1011 W/cm^2 focused intensity. In addition, we demonstrated that the surface plasmon generated this way also had extremely short, few-cycle duration (6-9 fs).

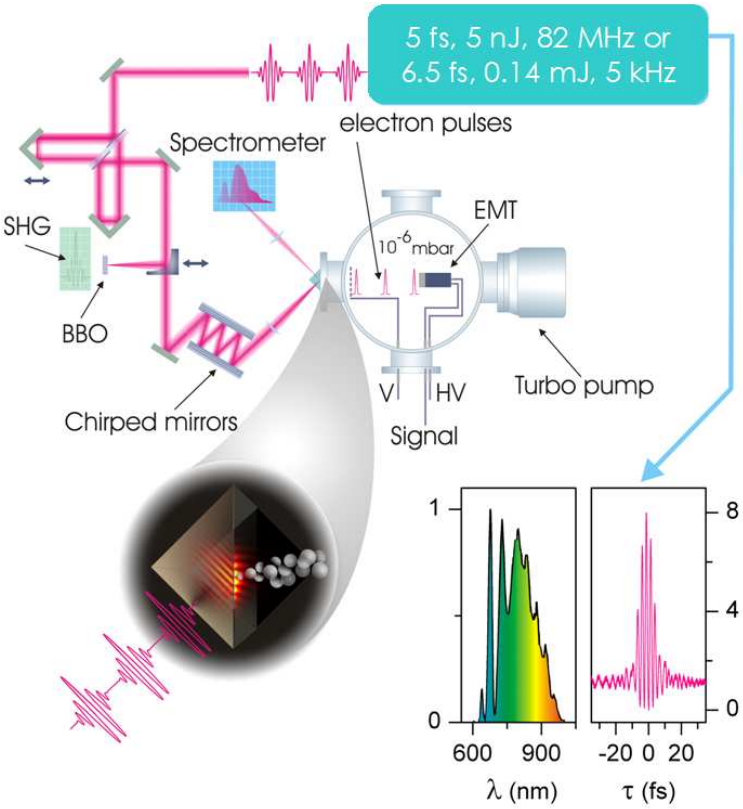

Fig. 1 *Scheme of the plasmonic electron acceleration setup with the main laser pulse parameters and pulse characterization results of a 5-fs, 5-nJ pulse (spectrum and second order autocorrelation are shown in the insets). SHG: second harmonic generation-based autocorrelation measurement, BBO: β-BaB_2O_4 second harmonic crystal, EMT: electron multiplier tube, HV: high voltage feedthrough, V: retarding grid voltage feedthrough. Pulse propagation in the prism material was pre-compensated for by introducing broadband chirped mirrors and finely tuneable dispersive elements (a pair of thin glass wedges) into the beam.*

Theoretical research. — Concerning above-threshold nonlinear photoelectric effect, in accord with our theoretical calculations, the broad energy spectra of surface plasmon mediated electron emission was also found experimentally. The results of these investigations support the physical picture offered by our concept of plasmon-induced oscillating near field of a double layer at the metal-vacuum interface. The electrons have been described by dressed quantum states (generalized Volkov states), which contain the

interaction with the plasmon field and the induced dipole interaction non-perturbatively. Similarly to the electron spectra, large deviations from the perturbative behaviour have also been found in the intensity dependence of the emitted fundamental and the second harmonic signals, even at moderate incoming laser intensities.

The wave function for a free particle in two dimensions and in a state with definite values of the energy and angular momentum shows some unusual effects (e.g. the appearance of quantum anti-centrifugal force). On the basis of the analytical study of the Wigner function, we have identified the origin of these subleties as interference in two-dimensional space where Huygens' principle breaks down.

Entanglement between two different kinds of interacting particles, photons and electrons has been analysed. The study of the time evolution of entanglement between the initially separated electron wave packet and a strong radiation mode led to the conclusion that in general there are non-vanishing entropy remnants in the subsystems after the interaction. The calculated values of the entropy remnants explicitly reflect back the irreversible character of the Compton process.

We have worked out a unified treatment of classic and recent Hanbury Brown and Twiss type counting experiments for both bosons and fermions. The new formalism relies on the Boole algebra of counting events and the associated classical probability space. In the framework of this description several two-point correlation experiments have been successfully described without the use of standard second quantization, even in the single-particle regime.

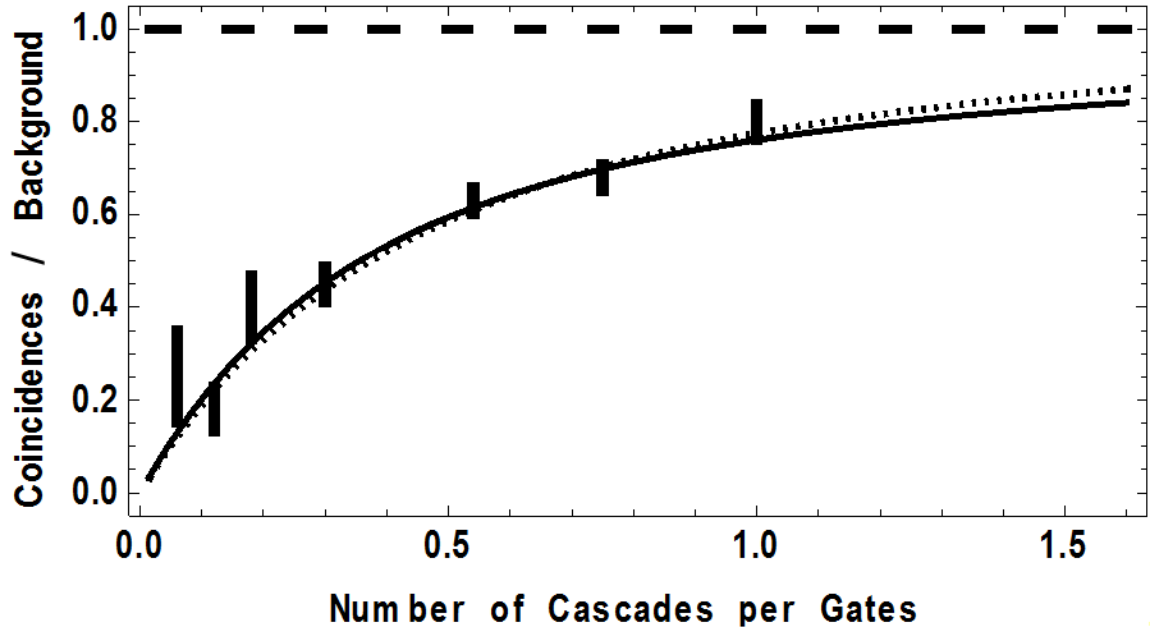

Fig. 2 *Photon anticorrelation curves displaying the normalized coincidences $\langle N_1N_2\rangle/\langle N_1\rangle\langle N_2\rangle$ in the single-photon regime.*

Fig. 2 shows the photon anticorrelation curves displaying the normalized coincidences $\langle N_1N_2\rangle/\langle N_1\rangle\langle N_2\rangle$ in the single-photon regime. In the experiment, the Hanbury Brown and Twiss type apparatus was pumped by the lower transition of an atomic cascade emission, while the upper cascade photons were used for triggering the two detectors. The rectangles represent the experimental data [Aspect, A.; Grangier, Ph.: Wave-particle duality for single photons. *Hyperfine Interactions*, **37**, 3-18 (1987)], and the dotted line shows the theoretical result, according to standard quantum mechanics. The full curve

corresponds to our theoretical formula derived on the basis of classical probability theory. Both the standard quantum description and our new formalism reproduce quite well the experimental results.

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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)

OTKA 60256 Investigation of femto- and attosecond light-solid interactions with controlled-waveform laser pulses, individual grant of the Hungarian Scientific Research Fund (P. Dombi, 2006-2010)

OTKA 72960 Ultrafast dynamics of surface plasmons, individual grant of the Hungarian Scientific Research Fund (M. Lenner, 2008-2011)

Marie Curie Reintegration Grant of the European Union (M. Lenner, 2008-2011)

Max Planck Institute for Quantum Optics (Garching, Germany), Surface plasmon research using STM (N. Kroó, M. Lenner), 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)

Vienna University of Technology, Photonics Institute, Austria, Experiments on surface plasmon enhanced electron acceleration with few-cycle laser pulses (P. Dombi, M. Lenner)

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)

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Other

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M. LASER PHYSICS

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

Gas discharge physics. — In a series of simulation studies by the Particle in Cell technique we have investigated basic processes in capacitively coupled radiofrequency discharges, which complemented experimental studies carried out at the Ruhr University, Bochum (Germany). The subjects of our studies have been: (i) the electron dynamics, formation of electron beams by sheath expansion, (ii) the charge dynamics in the sheath region, as well as (iii) the effect of secondary electrons on the separate control of ion energy and flux in dual-frequency capacitively coupled radio frequency discharges. Experimental studies have been carried out to clarify the effect of the anode material on the characteristics of glow discharges used in analytical spectroscopy. We have carried out a thorough comparison of the modeling approaches used for the description of low-pressure direct-current glow discharges. A heavy-particle hybrid model complemented with a set of equations of a complex external electrical circuit has been applied to describe the ignition of the discharge in plasma sources used in analytical chemistry.

Strongly coupled plasma research. — In single layer dusty plasma experiments we have realized a rapid temperature quench from liquid to solid state. Fast particle image velocimetry analysis revealed the details of the time evolution of the crystallite growth process in a two-dimensional Yukawa system. At very short times a rapid ordering was observed, which is due to the ballistic motion of the particles toward their local equilibrium position. Collective rearrangement of the small crystallites to form larger ones is a slower process, which can be well described with a power-law type growth of the average domain size in time. Particle level molecular dynamics simulations of two dimensional dipole and magnetized Yukawa systems, as well as 3D sheared Yukawa systems were performed. The external magnetic field results in the appearance of high harmonic Bernstein modes in the current fluctuation spectrum, although the frequencies appear shifted due to strong correlations of the underlying interacting particle ensemble.

Surface wave microwave discharge systems for biomedicine and nanostructuring. — Surfatron generated surface wave microwave discharges produced in small diameter tubes contain high density of active species. When the discharge is created in flowing gas the active species can be transported into different size and configuration reactors, that can be used for different applications, such as sterilization of medical tools, deposition of oxide films or oxide nanowires. 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 by means of modeling. The surface wave microwave discharge and the small volume afterglow is 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). — The ELCAD operates in a self-generated, saturated water vapor. The development mechanism and the main properties of this saturated water vapor were investigated. The ELCAD plasma was exposured by an Nd:YAG laser operating at a wavelength of 533 nm and at right angles to the exposure, the scattered light was measured by a CCD camera as a function of the time

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of exposure. In this way, the water molecule-cluster leaving the solution cathode could be observed and the mass of sputtered water could be studied as a function of discharge current and current density. In the case of a normal ELCAD, the mass of sputtered water was found to be about 150 mg/min with a current of 80 mA and a current density of 0.5 A/cm^2. The mass of sputtered water decreased with decreasing current. A current-threshold of 20-40 mA was found. For the currents lower than this threshold, the sputtering stops, but the discharge, however, is henceforward operating. This refers to that the electrons can leave the solution still at such low current also. This is in accordance with the current threshold observed in the occurrence of the emitted atomic metal lines. In the case of capillary (abnormal) type of ELCAD, the mass of sputtered water was found to be 1500 mg/min with a current of 80 mA and a current density of 3.7 A/cm^2. Using the same current and a copper cathode, the mass of sputtered copper is only 0.5 mg/min. The comparison of these data shows that the ELCAD operates in a self-generated saturated water vapor.

Imaging ellipsometer. — The first unit of our new type of multispectral imaging ellipsomters was successfully finished, tested, in cooperation with the Research Institute for Technical Physics and Materials Science HAS, and it is ready to be installed in the USA.

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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)

OTKA F 67556 Modelling of post-discharges used for sterilization and surface treatment (K. Kutasi, 2008-2010)

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

HAS-NSF/102 Advanced numerical modeling of strongly coupled many-particle systems (Z. Donkó, 2008-2010)

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

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M.22. Horváth ZGy; 50 éves a lézer I-II. (50 Years of Laser I-II, in Hungarian); *Természet Világa*; **141**, 447, 2010; **141**, 503, 2010

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M.23. Kutasi K, Pintassilgo* CD, Guerra* V, Sá* PA, Loureiro* J, Moisan* M; Flowing plasma-afterglow as a promising sterilization medium; *Proceedings of the XXth European Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG), 13-17 July 2010, Novi Sad, Serbia*; Eds.: Z.Lj. Petrovic, G. Malovic, D. Maric, Institute of Physics, Belgrade, Serbia; WPM_02, pp. 1-2

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M.25. Schulze J, Schüngel* E, Donkó Z, Czarnetzki* U; Charge dynamics in capacitively coupled radio frequency discharges; *Proceedings of the XXth European Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG), 13-17 July 2010,*

Novi Sad, Serbia; Eds.: Z.Lj. Petrovic, G. Malovic, D. Maric, Institute of Physics, Belgrade, Serbia; P2.59, pp. 1-2

M.26. Schulze J, Schüngel* E, Donkó Z, Czarnetzki* U; Excitation dynamics in electrically asymmetric capacitively coupled radio frequency discharges - Experiment, simulation, and model; *Proceedings of the XXth European Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG), 13-17 July 2010, Novi Sad, Serbia;* Eds.: Z.Lj. Petrovic, G. Malovic, D. Maric, Institute of Physics, Belgrade, Serbia; P3.23, pp. 1-2

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M.28. Hartmann P, Donkó Z, Kalman* GJ, Kyrkos* S, Golden* KI, Rosenberg* M; Collective dynamics of complex plasma bilayers; *Proceedings of the XXth European Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG), 13-17 July 2010, Novi Sad, Serbia;* Eds.: Z.Lj. Petrovic, G. Malovic, D. Maric, Institute of Physics, Belgrade, Serbia; P3.03, pp. 1-2

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M.30. Derzsi A, Donkó Z; Modeling of the ignition of low-pressure glow discharges; *Proceedings of the XXth European Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG), 13-17 July 2010, Novi Sad, Serbia;* Eds.: Z.Lj. Petrovic, G. Malovic, D. Maric, Institute of Physics, Belgrade, Serbia; P2.42, pp. 1-2

M.31. Donkó Z; Particle simulation methods for studies of low-pressure plasma sources; *Proceedings of the XXth European Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG), 13-17 July 2010, Novi Sad, Serbia;* Eds.: Z.Lj. Petrovic, G. Malovic, D. Maric, Institute of Physics, Belgrade, Serbia; GLCR, pp. 1-4

Patent

M.32. Horváth Z Gy, Juhász* G, Fried* M, Major* C, Petrik* P; Imaging optical device with a pinhole camera; US 12/601,410 (USA); 2010-508-914 (Japan)

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. — In the frame of the Extreme Light Infrastructure (ELI) FP-7 ESFRI project we participated in the planning of the *Attosecond Laser facility* to be built in Hungary (ALPS). We contributed to the design of the block diagrams of the facility, specification and parameterisation of the main parts, elaboration of the optical testing and measurement technologies etc. We participated in the preparation of the final report and several chapters of the White Book of the project. The ALPS facility would serve to perform ultrafast attosecond studies of laser-matter interaction, afford wide benefits to society ranging from improvement of oncology treatment, medical imaging to fast electronics. Within this project in which most European countries are involved, we are participating in almost all Work Packages; our department is responsible for Optical Metrology and Optical Coatings. At different WP meetings, Participating Countries Council Meetings and Steering Committee Meetings (we organised several of them in Budapest) we made a dozen of presentations and discussed our possibilities and responsibilities in different tasks to be developed and a number of experimental applications. We participated in the development of interferometric and light scattering methods, vibration analysis and alignment control, investigation of the optical quality of the substrates and crystals and production of special optical coatings.

We further developed and tested the portable industrial version of the *dual wavelength optical particle analyzer* (DWOPS) enabling simultaneous measurement of the concentration, size distribution, refractive index and absorption of the aerosol particles in the red mud measurements at hot spots in Devecser and Kolontár where the environmental disaster was happened. In this area during measurement campaigns we collected samples for laboratory analysis - study of morphology, Raman spectra, luminescence, etc. Based on the above mentioned studies we discovered several new properties of the air contamination from the 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 airways and determined deposition parameters for different other types of contaminations.

In the frame of Jedlik Ányos project the DWOPS was also utilized in 3 different longer measurement campaigns that aims to develop a new method/model for identification of different aerosol sources having different origin (anthropogenic – industrial, combustion/traffic, agricultural, red mud, etc.). The main advantage of the new method is that with a short (several minutes) sampling time the contamination sources could be determined without further time consuming and expensive laboratory analyses. Fig. 1 shows the results obtained using DWOPS and a black carbon Aethalometer, where the data from different instruments are compared. A good agreement between the results observed by different instruments can be observed.

We started the design of a *pulmonary waveform generator* for in vitro testing and measurement of the aerosol flow in transparent hollow human airway models. The computer controlled pneumatic system enables the generation of any breathing waveform with different air flow parameters. This system is connected with a hermetic transparent

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chamber holding the lung models and enabling optical measurements using Laser Doppler Velocimetry (LDV).

This complex system is planned to utilize for the verification of the numerical stochastic lung models to give valuable information on aerosol drug or contamination deposition in different generations within human lung.

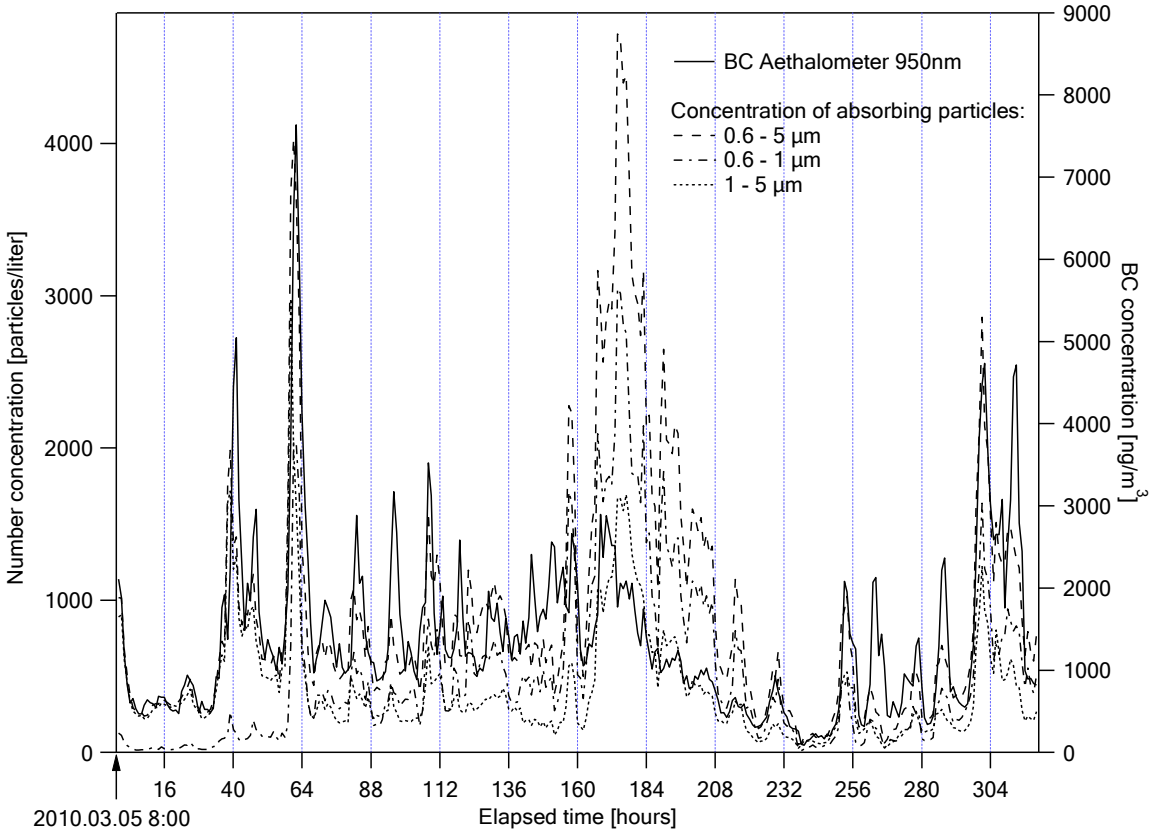

Fig. 1 *Comparison of Dual Wavelength Optical Particle Spectrometer (DWOPS) and APC instruments data of different aerosol sources*

We elaborated a method for study of the *statistics of photons* generated in different nonlinear optical processes based on measurement of cross-correlation functions with high time resolution. Using these techniques we determined the statistics of light generated by surface plasmons (SP) and compared it with the statistics of the incident light. The great advantage of this method is the independence on the intensity fluctuations of the incident excitation light. The temporal statistical behaviour of SP emitted photon generated at different excitation intensities where determined.

The research activity of this year was concentrated to the development of Nano-LDA *photon correlation system*, under KMOP project and Technoorg Linda Ltd. - SZFKI contract. Cold testing, calibration and implementation of opto-mechanical unit and measurement data collection hardware and software are currently being developed. First measurements on real 100 nm particles were obtained and reported. The online, simultaneous velocity, size and concentration measured data obtained for single particle transit was credibly corresponding to input data. Design, construction and manufacturing of the prototype Nano-LDA photon correlation system are currently being executed.

Amorphous carbon layers. — Coatings are of great importance for medical implants. They could be used for the improvement of functional characteristics of the implant and/or to promote the appropriate host response after the implantation. The second aim could be

achieved by the utilization of passive or active protective coatings. The passive layer separates the toxic/inert/non-tissue friendly implant material from tissues. The active (or drug eluting) coatings contain drugs promoting the healing and regeneration of the tissue in the vicinity of the implant, while minimizing the risk of side-effects. Earlier we have developed a protective amorphous carbon coating for stents – tubular metallic meshes implants used for elimination of occlusions and narrowing of the blood vessels (e.g. coronary disease) – and the research was continued by the preparation of a drug eluting active coating.

The key issues of implant coatings are their biocompatibility, uniformity, and appropriate physical characteristics that will not worsen the properties of the implant itself. In our case a hydroxyethyl methacrylate (HEMA) based hydrogel was selected for drug-eluting matrix that is proven to be biocompatible and elastic enough to withstand the deformation during the stent expansion. The optimized monomer mixture consisted of 30 vol.% HEMA, 65 vol.% water and 5 vol.% of diethylene glycol dimethacrylate (DEGDMA), a crosslinking agent enhancing the mechanical properties of the polymer.

The formation of the hydrogel layer was examined on metal surfaces both bare and coated with amorphous carbon. After coating the substrate surface with a monomer mixture, the polymerization was performed by a 10 kGy dose of γ-radiation from a ^{60}Co γ-source.

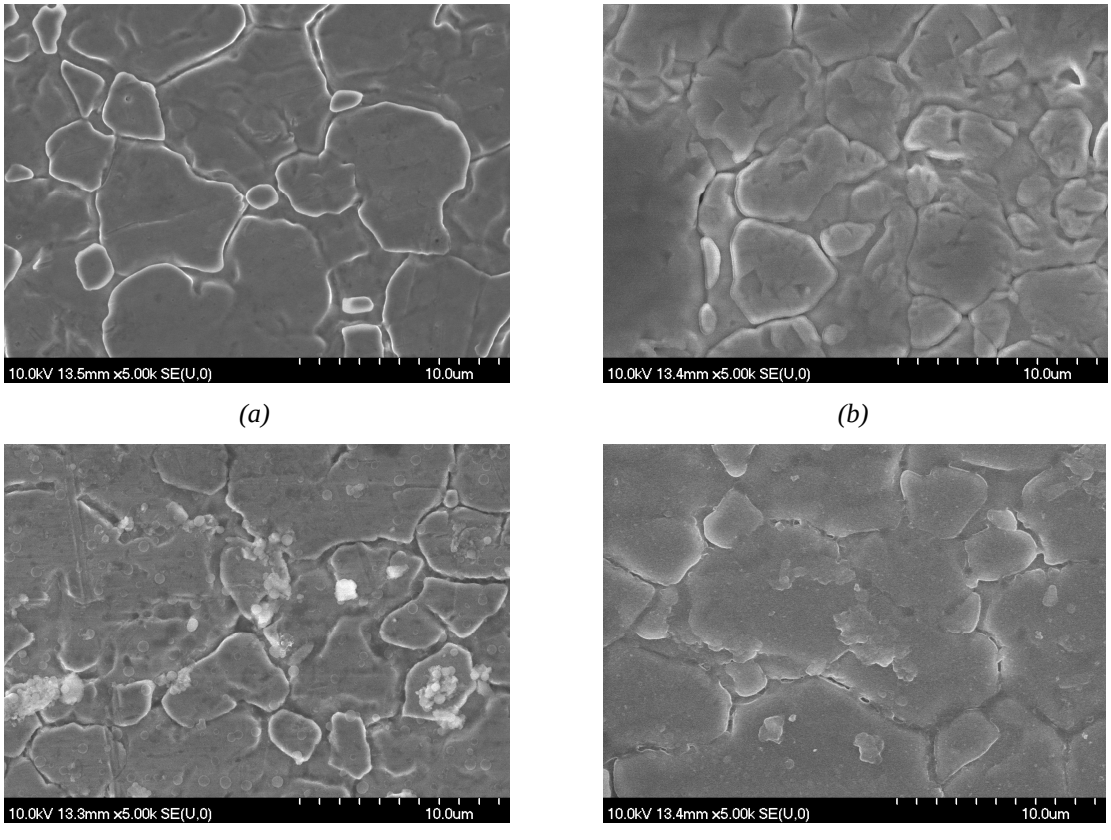

Fig. 2 *SEM pictures of (a) bare Inconel surface, (b) a-C:H coated on Inconel surface, HEMA hydrogel layer on (c) metal and (d) amorphous carbon.*

Fig. 2 compares the scanning electron micrographs of bare Inconel substrate, metal coated with a-C:H thin film and the hydrogel layers formed on these two substrates. It can be seen that polymer layers were formed on top of both substrates, but their morphology differs remarkably. While the coverage is continuous in both cases, the layer is not uniform on the

alloy surface: spherical shapes can be seen on the SEM picture indicating the uneven distribution (clotting) of the monomer mixture. On a-C:H the polymer is much more uniform. Contact angle measurements showed perfect wetting of the latter surface by the monomer mixture, while less wetting was observed on bare metal surface, even after treating it with Ar, H_2O and N_2 plasmas.

The presence of the hydrogel layer on top of bare and a-C:H coated metal surfaces was confirmed also by Raman spectroscopy (Fig. 3), which gave information on the bonding configuration of the amorphous carbon layer, too.

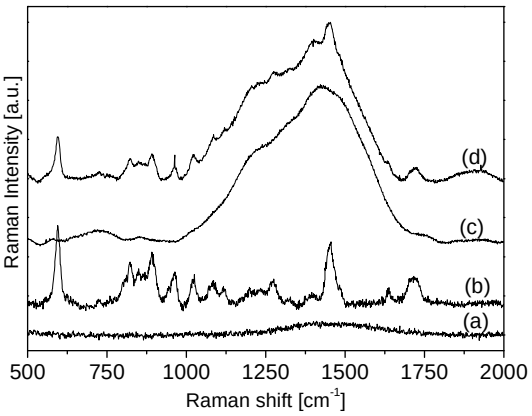

Fig. 3 *785 nm excited Raman spectra of (a) bare metal substrate, (b) the hydrogel, (c) a-C:H layer on metal substrate and (d) HEMA hydrogel on top of a-C:H. The relatively low intensity of the polymer peaks compare to those of a-C:H is due to the significantly lower scattering cross-section of the former.*

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Grants and international cooperations

IAEA-15455 Porous polymer drug-eluting coating prepared by radiation induced polymerization (M. Veres, 2009-2010)

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

Gi3989/2008 Technoorg-Linda Ltd. - SZFKI, Development of nanoparticle mesurement system, (P. Jani, 2009-2011)

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, 2007-2010, 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, 2007-2010)
410/EAC EAC Conference (A. Czitrovszky, 2010)
MTA SZFKI-Envi-Tech Ltd. Gi 5492/2010 Co-operation Contract (A. Czitrovszky, 2010)
TÉT KR-6/2009 Hungarian Korean bilateral Intergovernmental cooperation Surface modification of nanodiamond by conductive polymer (M. Veres, 2010-2011)
HAS-RAS Hungarian Russian Academic co-operation (A. Czitrovszky, 2008-2011)

Long-term visitors

— Prof. Mitsa Vladimir, Uzhgorod State University, Uzhgorod, Ukraine, August 15 – September 15, 2010 (host: M. Koós)

Publications

Articles

N.1. Vámos L, Jani P; Nanoparticle sizing algorithm for photon correlation LDA; *Optical Engineering*; **49**, 1, 2010

N.2. Veres M, Perevedentseva* E, Karmenyan* AV, Tóth S, Koós M; Catalytic activity of gold on nanocrystalline diamond support; *Phys Stat Sol*; **7**, 1211–1214, 2010

N.3. Kondrat* O, Popovich* N, Holomb* R, Mitsa* V, Petrachenkov* O, Koós M, Veres M; Ab initio calculations and the effect of atomic substitution in the Raman spectra of $As(Sb,Bi)_2S_3$ films; *Phys Stat Sol*; **7**, 893-896, 2010

N.4. Holomb* R, Mitsa* V, Johansson* P, Veres M; Boson peak in low-frequency Raman spectra of As_xS_{100-x} glasses: nanocluster contribution; *Phys Stat Sol*; **7**, 885–888, 2010

N.5. Lukács* R, Veres M, Shimakawa* K, Kugler* S; On photoinduced volume change in amorphous selenium: Quantum chemical calculation and Raman spectroscopy; *J Appl Phys*; **107**, 073517, 2010

N.6. Horváth* A, Balásházy* I, Farkas* Á, Sárkány* Z, Dobos* E, Czitrovszky A, Hofmann* W; Computer simulation of airway deposition of intact and fragmented pollens; *International Journal of Environmental Health Reasarch*; accepted for publication

N.7. Bereznai* M, Budai* J, Hanyecz* I, Kopniczky* J, Veres M, Koós M, Tóth* Zs; Spectroscopic ellipsometry of nanostructured carbon films deposited by pulsed laser deposition; *Thin Solid Films*; accepted for publication

N.8. Gelencsér* A, Kovács* N, Turóczi* B, Rostási* Á, Hoffer* A, Imre* K, Nyírő-Kósa* I, Csákberényi-Malasic*s D, Tóth* Á, Czitrovszky A, Nagy A, Nagy* Sz, Ács* A, Kovács* A, Ferincz* Á, Hartyán*i Zs, Pósfai* M; The red mud accident in Ajka (Hungary): caracterization and potential health effects of fugitive dust; *Env Sci Technol*; accepted for publication in.

Conference proceedings

N.9. Oszetzky D, Nagy A, Kerekes A, Czitrovszky A; Aerosol concentration measurement by laser light scattering; In: *International Conference on Advanced Laser Technologies ALT'10, Egmond aan Zee, The Netherlands, September 11-16, 2010*; p. 180-181, 2010

N.10. Czitrovszky A; Interferometry applied to ELI Attosecond Facility; In: *International Conference on Advanced Laser Technologies ALT'10, Egmond aan Zee, The Netherlands, September 11-16, 2010*; p. 64-65, 2010

N.11. Kerekes A, Nagy A, Czitrovszky A, Oszetzky D; Air flow measurements with a realistic transparent hollow airway model; In: *International Conference on Advanced Laser Technologies ALT'10, Egmond aan Zee, The Netherlands, September 11-16, 2010*; p. 134-135, 2010

N.12. Veres M, Koós M, Tóth S, Himics L; Sp2 carbon defects in nanocrystalline diamond detected by Raman spectroscopy; In: *IOP Conference Series: Materials Science and Engineering: Proceedings of the 11th Europhysical Conference on Defects in Insulating Materials, 12-16 July, 2010, Pécs, Hungary;* accepted for publication

Book chapter

N.13. Czitrovszky A; Application of optical methods for micron and sub-micron particle measurements, Chapter 7; In: *Aerosols - Science and Technology*; Ed.: I. Agranovski, J Wiley; pp. 203-241, 2010

O. FEMTOSECOND LASERS

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

Continuing our research on **dispersive mirrors**, we showed that the reflection group delay as well as the absorption/scattering loss of a dielectric multilayer mirror is proportional to the energy stored by the standing wave electromagnetic field built-up in such 1D photonic bandgap devices.

We examined three different highly reflective (HR) multilayer mirror structures to demonstrate the proportionality of the reflection group delay as well as the (absorption or scattering) loss to the stored energy. We used the well known matrix method to calculate the standing wave electromagnetic field inside the multilayer structure.

The first example is a simple quarter-wave (QW) stack with a reference vacuum wavelength of λ_0 = 800 nm comprising 10 pairs of low and high index layers: $S \mid (HL)^{10} \mid A$. The refractive index of the substrate (S) is n_s = 1.51, the refractive index of air (A) is n_A = 1.00. H and L denote the high and low refractive index layers of $\lambda_0/4$ optical thicknesses, respectively, where n_H = 2.315 and n_L = 1.45. The second example is an ultra-broadband chirped mirror (UBCM) design, first we reported in 1997. We note that these kinds of UBCM-s are now used for dispersion control and feedback over an octave bandwidth. The third structure we investigated is a multi-cavity Gires-Tournois interferometer (MCGTI) mirror. Here n_H = 2.026, n_L = 1.48, n_S = 1.51, n_A = 1.00. This specific mirror design provides a huge negative GDD of -1200 fs^2 over a spectral bandwidth of ~50 nm, which can be explained by the extremely high energy stored in the multilayer structure.

In order to illustrate the point that the wavelength dependent energy storage determines both dispersive and loss properties of dielectric high reflectors, we show the computed stored energy spectral density for a standard quarter-wave multilayer mirror design, an ultra-broadband chirped mirror design and a highly dispersive MCGTI mirror design in Fig. 1a, Fig. 1b and Fig. 1c, respectively.

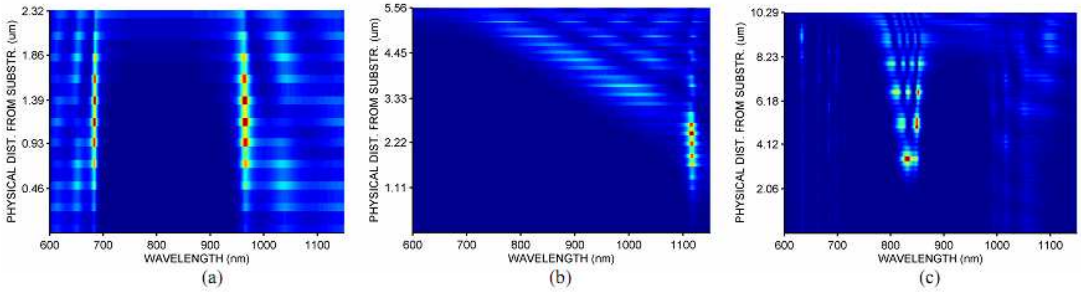

Fig. 1 *Computed stored energy spectral density in (a) a standard quarter-wave multilayer mirror design, (b) an ultra-broadband chirped mirror design and (c) a highly dispersive MCGTI mirror design*

The computed group delay vs. wavelength, energy stored vs. wavelength and absorption vs. wavelength functions are plotted in Fig. 2a, Fig. 2b and Fig. 2c, respectively. For calculating the absorption/scattering loss, we expected a uniform absorption coefficient all over the layer structures, which can be expressed by the complex refractive index in the form of: $\tilde{n} = n - ik$. For each layer, a realistic k = 0.0001 value was used. It can be clearly seen that higher group delay, which is proportional to the energy stored by the standing wave field, goes together with an increased absorbed (or scattered) power. This fact may

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considerably reduce the damage threshold of highly dispersive MCGTI mirrors compared to standard, low dispersion, quarter wave mirror designs.

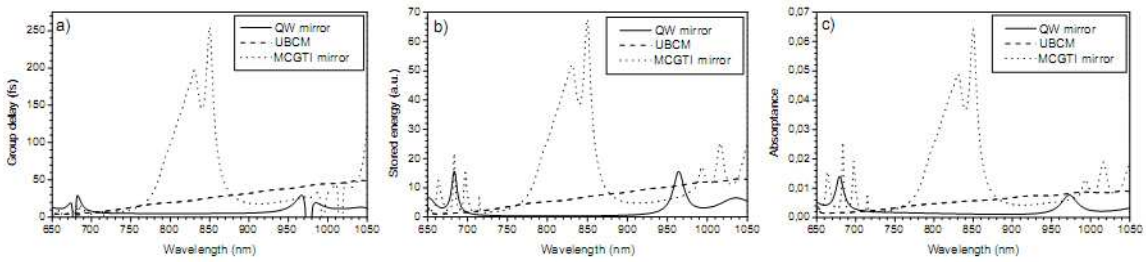

Fig. 2 *Computed (a) group delay vs. wavelength, (b) energy stored vs. wavelength and (c) absorption vs. wavelength functions of a standard quarterwave multilayer mirror design (continuous line), an ultra-broadband chirped mirror design (dashed) and a highly dispersive MCGTI mirror design (dotted)*

Concluding these results, we can say that the application of highly dispersive mirrors in high power femtosecond laser systems requires advanced coating deposition technologies such as ion-beam or magnetron sputtering resulting in dense, extremely low absorption and scattering loss multilayer coatings on super-polished substrates. In spite of these efforts, damage threshold problems may still arise for highly dispersive mirrors in high peak power laser systems.

In collaboration with R&D Ultrafast Lasers Ltd, we have developed a **broadly tunable, long-cavity**, low-pump-threshold, **pulsed Ti:Sapphire laser**. 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, being ideal for nonlinear microscopy. The schematic of the laser setup is shown in Fig. 3.a.

The laser can be easily mode-locked with the soft aperture Kerr-lens mechanism. In our current setup, the wavelength could be tuned over a 115 nm wide range between 745 nm and 860 nm, in mode-locked operation without changing cavity optics except the output coupler ("SW OC" for the 745-820 nm range and "MW OC" for the 785-860 nm range). Fig. 3.b. shows the measured average output power versus wavelength function. The maximum of the measured average output power was 200 mW (at 800 nm), which corresponds to a pulse energy value of 10.2 nJ at 19.6 MHz repetition rate. The measured second-order autocorrelation trace indicates nearly transform-limited pulses with pulse duration of ~140 fs.

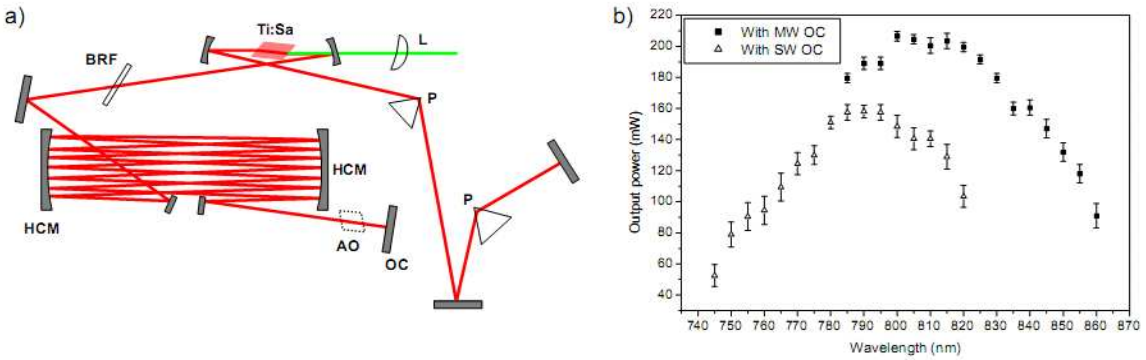

Fig. 3 *(a) Setup of the long-cavity oscillator. L: pump focusing lens, Ti:Sa: titanium-sapphire crystal – the path length in the crystal is 4 mm. BRF: birefringent filter for wavelength tuning. P: prism, HCM: Herriott-cell mirror, OC: output coupler. AO: Acousto-optic modulator for regenerative modelocking (only inserted in the cavity when the laser is modelocked by regenerative modelocking). (b) Output power versus wavelength at a pump power of ~2.5 W. Two different output couplers were used for the short wavelength part (SW OC) and for the long wavelength part (MW OC).*

In order to reduce the reflection losses in the cavity, and extend the tuning range of our long cavity laser, extremely low reflection loss ion beam sputtered (IBS) ultra-broadband chirped dielectric mirrors were used to build a slightly modified cavity. The mirrors were developed by R&D Ultrafast Lasers Ltd and were manufactured in the USA. Application of the new cavity mirrors resulted in a lower pump threshold and a higher output power of the laser. Currently we have efforts focusing to extend the tuning range up to the 680-1040 nm regime at similar pump power levels.

Concluding our result on this topic, we dare say that we have developed a new laser concept for a low repetition rate, ultrashort pulse (τ < 150 fs), tunable laser source being pumped at moderate pump powers. These features result in a higher signal to noise ratio, a lower photo-induced degradation of the biological samples and a more cost efficient construction than its 80 MHz predecessors, and hence this laser construction is ideal for nonlinear microscopy applications.

In the summer of 2010, we built **two new laboratories**: one for development of *femtosecond pulse fiber lasers and fiber optic parametric oscillators* (FOPO-s) and one for *nonlinear microscopy*. In the fiber optics laboratory, we are focusing on development and application of our newly developed inversed dispersion slope solid core photonic bandgap (PBG) fibers exhibiting anomalous dispersion over most of the bandgap. In the nonlinear microscopy laboratory, we use a new, commercial Zeiss Axio Examiner two-photon absorption fluorescence microscope to take sub-micron resolution 3D pictures of different biological samples.

Among others, this year we made a solid core photonic bandgap design for dispersion compensation of our new *FemtoFiber* femtosecond pulse fibre oscillator/amplifier system (product of R&D Ultrafast Laser Ltd), whose picture is shown in Fig. 4. The computed dispersion function and transmission loss of an optimized fibre structure are shown in Fig. 5a, while the effective refractive index and effective core area vs. wavelength functions are plotted in Fig. 5b. The zero dispersion point is at 1077 nm in this specific case, which can be easily shifted by rescaling the fibre geometry. The compressed output of the fibre laser is currently used as a cost efficient femtosecond pulse laser source for nonlinear microscopy, including two-photon absorption fluorescence microscopy, second-harmonic generation (SHG) microscopy and coherent anti-Stokes Raman (CARS) microscopy.

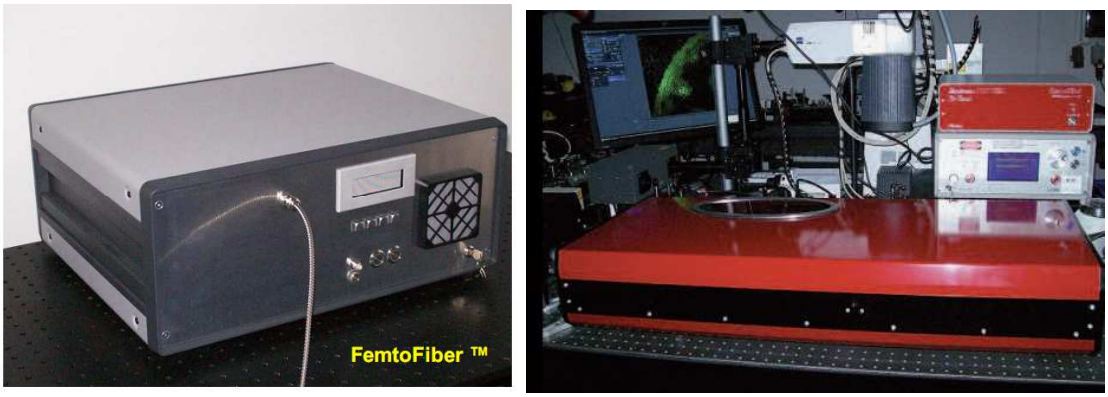

Fig. 4 *Photos of (a) our new, femtosecond pulse FemtoFiber ytterbium fibre oscillator/amplifier system and (b) our upgraded FemtoRose 100 TUN NoTouch Ti:sapphire laser used as laser sources for the new Zeiss Axio Examiner microscope. Both lasers can be fully controlled by the ZEN software of the microscope (fully hands free operation).*

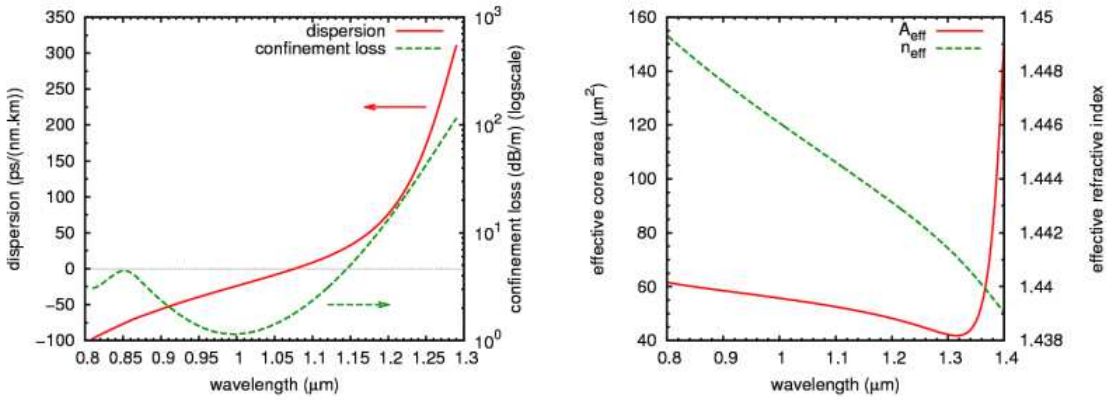

Fig. 5 *(a) Dispersion and confinement loss vs. wavelength functions and (b) effective refractive index and effective core area vs. wavelength functions of our new solid core photonic bandgap fibres developed for dispersion compensation of our femtosecond pulse ytterbium fiber oscillator/amplifier system shown in Fig. 4 (a).*

After some basic tests performed on the new Zeiss microscope, we tested some biological samples of our scientific interest in collaboration with researchers at the Department of Dermatology, Semmelweis University, Budapest. We are focusing on the question whether laser radiation from pulsed lasers such as femtosecond pulse Yb fiber lasers or Ti:sapphire **lasers do have any irreversible effect on the skin** when these lasers are used for taking 3D *in vivo* images of the skin by different nonlinear methods at different power levels and wavelengths. To this end, skin cells of mice have been exposed to UVB radiation (positive control) causing CpD mutation formation in DNA. To detect CpD islet we performed immunohistochemistry.

Specific 1st antibody raised against CpD molecules was applied in combination with a 2nd antibody that was conjugated with a fluorescent dye (Alexa 514) for 2P detection using Ti:Saphire laser. To prove specificity of the labeling we performed 1st antibody control. In this case immunohistochemistry was performed applying only Alexa labeled 2nd antibody staining. Signal missing nuclear staining in 1st antibody control proved that positive control recognized specifically CpD islet in chromosomes.Pictures could be made at a moderate laser powers below 5mW either from our Yb fiber laser operating at 1030 nm or from our tunable Ti:sapphire laser. In Fig. 6, we show two pictures of *in vitro* mice cells taken by the Zeiss Axio Examiner microscope.

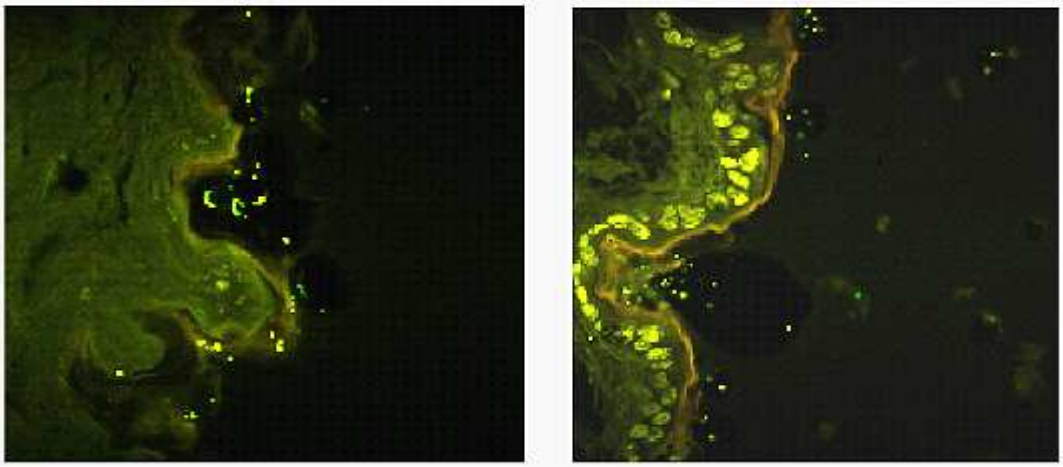

Fig. 6 *UVB induced CpD formation in nucleus of mice skin cells. Left: 1st antibody control. Right: positive control*

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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)

Contract

SZFKI-R&D Ultrafast Lasers Ltd: Development of a tuneable, long cavity Ti:sapphire laser for nonlinear and time resolved studies (Coordinator: R. Szipőcs, 2009-2010)

Publications

Conference proceedings

O.1. Antal P, Szipőcs R; Relation between group delay and energy storage in dispersive dielectric mirror coatings; In: *Advanced Solid State Photonics Conference;* OSA Technical Digest Series (Optical Society of America, 2010); Paper AMB17, 2010

O.2. Szipőcs R, Antal P; Relation between group delay, energy storage and absorbed/scattered power in highly reflective dispersive dielectric mirror coatings; In: *Optical Interference Coatings* (OIC) (Optical Society of America, 2010); Paper FB3, 2010

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 of nanooptically thin layers for advanced applications in laser physics and information technology. We have further refined our electron-beam deposition technology for producing of optical coatings containing nanooptically thin titania, tantala, hafnia, yttria, zirconia, alumina and silica layers. Using multiple target thin film optimisation method, we have developed low dispersion wide-band enhanced infrared silver reflectors (R >98%, 700 – 3000 nm, 45°) for OPO (Optical Parametric Oscillator) applications, new type low-dispersion wide-band beam splitters for high power ultrafast application using our superpolished Ø50.8 mm fused silica plates as substrates. Our indium-tin-oxide (ITO) layers having prescribed electrical resistance in the 13 – 16 ohm range were successfully applied as heatable windows in military vehicles. Our high damage threshold antireflective coatings are used in THz research at Massachusetts Institute of Technology. We have developed the electron-beam deposition technology for producing oxide-free, hard boron films useful in new type neutron detector devices.

Superpolishing technology. — We have continued our new project concerning the development of advanced optical polishing technologies for producing very smooth (lower than 0.4 nm rms surface roughness) borocrown glass and fused silica surfaces. We have demonstrated 0,34 nm rms surface roughness on our large size (250 x 80 mm) BK7 glass substrates superpolished with zirconia based polishing formulas manufactured by nanotechnological methods. The combination of superpolishing technology with ion-assisted deposition technology will open the door for producing very low loss and high damage threshold laser mirror coatings on large size substrates useful in the femtosecond petawatt laser facilities planned in the frame of the European project ELI.

Optical coatings for solar cell application. — We have continued our research project concerning the development of selective dichroic mirrors suitable for the modification of the reflected colour of amorphous silicon based solar cells resulting a better colour comfort feeling. Our new two component dichroic mirrors (blue, green and red reflectors) for the modification of colour appearance of the silicon solar cells without decreasing the efficiency can be used on the protective float-glass plates or directly on the silicon surfaces, too.

These results were obtained in the frame of the scientific cooperation between the Institute and Optilab Ltd.

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Contract

OPTILAB-SZFKI No. 0515/2010

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)

Q. GROWTH AND CHARACTERIZATION OF OPTICAL CRYSTALS

I. Földvári, L. Bencs, E. Beregi, G. Dravecz[#], K. György[#], Á. Péter, K. Polgár, Zs. Szaller

Growth and study of nonlinear borate crystals. — Rare earth (RE) doped $YAl_3(BO_3)_4$ (YAB) single crystals were grown by the top-seeded flux technique. High resolution Fourier transform (FT) spectroscopy (0.04 cm^{-1}) was employed to determine the term diagram of Tm^{3+} and Tb^{3+} ions in the crystal field of YAB. Six transitions were identified in the YAB:Tm crystals from the $^3H_6$ ground state of the Tm^{3+} ions to the $^3F_4$, $^3H_5$, $^3H_4$, $^3F_3$, $^3F_2$, and $^1G_4$ manifolds. All of their Stark components were assigned by using the temperature dependence (9-100 K) of the absorption lines. The low temperature spectra consists of sharp lines, broadened ones and those split to components. These features were attributed to Tm-Tm interaction and optical hyperfine structure. The Tm-Tm interaction was already significant in the 1 mole% Tm crystal. The half-width (FWHM) of the Tm^{3+} absorption lines was typically around 0.5 cm^{-1} at 9 K for the 0-0 transitions, and gradually broadens towards the intrinsic absorption edge.

In YAB:Tb crystals the crystal field splitting of the fundamental $^7F_6$ and the excited $^7F_5$, $^7F_4$, $^7F_3$, $^7F_2$, $^7F_1$, $^7F_0$, and $^5D_4$, manifolds of the Tb^{3+} ions have been experimentally determined and fitted with a single Hamiltonian crystal field calculation. All of the possible Stark components were observed in the spectra, and the ground state splitting was derived from the temperature dependence of the spectral lines. The model calculations were in good agreement with the experimental data concerning the energy levels and the polarization of the transitions obsereved in the linar dichroism measurements. The free ion and crystal field parameters of the system were calculated. The thermal shift of the spectral lines were used to determine the electron-phonon interaction, and the related model fitting suggested the evidence of single phonon coupling.

Optical absorption, excitation and luminescence spectra were recorded for Sm-doped YAB crystals in the visible range at 10 K and 300 K. In the excitation spectra the $^6H_{5/2}\rightarrow{}^4G_{5/2}$ and the $^6H_{5/2}\rightarrow{}^4F_{3/2}$ transitions were dominant. After both excitations the $^4G_{5/2}\rightarrow{}^6H_{5/2}$, $^4G_{5/2}\rightarrow{}^6H_{7/2}$ and $^4G_{5/2}\rightarrow{}^6H_{9/2}$ emissions were prominent, and the $^4G_{5/2}\rightarrow{}^6H_{11/2}$ emission was also detectable. The fine structure of the luminescence transitions well corresponded to the Stark components of the terminating levels. According to the Judd-Ofelt calculations the branching ratio to these $^6H_{5/2}$, $^6H_{7/2}$, $^6H_{9/2}$ and $^6H_{11/2}$ levels were 7.4%, 75.7%, 13.6% and 3.3%, respectively, for the π-polarized spectrum, and slightly different for the σ-polarized one. The lifetime of the $^4G_{5/2}$ level was relatively long (2 ms at rooom temperature). The narrow luminescence line, the high branching ratio and the long excited state lifetime make the $^4G_{5/2}\rightarrow{}^6H_{7/2}$ Sm^{3+} transition promissing for laser effect in YAB:Sm. The $^6H_{7/2}$ level is separated from the ground state $^6H_{5/2}$ by about 1100 cm^{-1} which is suitable for four-level laser operation.

Growth and study of scintillator crystals. — Surface dissolution has been investigated on {100}, {010}, {001}, {110} and {101} oriented $Lu_{1.6}Y_{0.4}SiO_5$:Ce crystal samples by using orthophosphoric acid up to 180 °C. Depending on the etching temperature and surface orientation smooth or bunched surfaces were produced. The transition temperature between smooth and bunched etching was found between 150-160 °C. The surface dissolution rate was the highest on {110} oriented faces. In order to study the effect of the etching process on the scintillation properties, temperature dependent optical absorption

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measurements were carried out up to 236 °C. Depending on the post-growth history of the sample, low temperature annealing treatments (like chemical etching in orthophosphoric acid below 200 °C) may influence the scintillation mechanism by modifying the concentration of shallow traps.

Growth and study of lithium niobate crystals with different compositions and doping. — Stoichiometric $LiNbO_3$ crystals were grown with Sc_2O_3, In_2O_3 and ZrO_2 dopants in different concentrations. Dopant incorporation and the defect structure were characterized by the UV-VIS-IR absorption method. Photo-induced refraction change was followed by the Z-scan method. These investigations revealed that both indium and scandium dopants improved the optical damage resistance of the crystals, but the performance of the zirconium doped crystal was below the expectation.

Growth and study of bismuth tellurite (Bi_2TeO_5) crystals. — Single crystals of Bi_2TeO_5 were grown by the Czochralski technique. High resolution FT spectroscopy was applied to investigate the Tb^{3+}-dopant related absorption spectra. Five infrared transitions were identified from the $^7F_6$ ground state to the $^7F_4$, $^7F_3$, $^7F_2$, $^7F_1$, and $^7F_0$ manifolds. The only visible transition not covered by the host absorption was the $^7F_6 \rightarrow {}^5D_4$. Following the temperature dependence of the spectra, the detailed term diagram of the Tb^{3+}-manifolds was established. All the predicted Stark components were identified in the transparent range of the crystal. The temperature dependence of the spectra was also applied to derive some of the Stark components of the $^7F_6$ ground state. The fine structure of the spectral lines is in accordance of a dominantly single site incorporation model to one of the Bi-sites.

Development of analytical methods for materials science and environmental control. — Analysis of daily, size-segregated aerosols (fine, medium, and coarse) was performed by EDXRF to provide their elemental composition and to study their seasonal variation at a coastal spot of the Belgian North Sea (De Haan). The elemental content of each sample/aerosol fraction could be associated with the main (prevailing) air-masses. The Cl, Si and S content was found to be proper tracers to map the seasonal differences in the aerosol content. Daily and seasonal variation in the organic carbon (OC), elemental carbon (EC), elemental (metal) content and mass of fine aerosols ($PM_{2.5}$) were studied in Northern Belgium. Continuous, semi-continuous and non-continuous methods of $PM_{2.5}$ mass monitoring were critically evaluated. The average metal content was 2-6 % of the total $PM_{2.5}$ mass. The total carbon (EC+OC) content of $PM_{2.5}$ ranged between 3-77 % with averages of 12-32 %, peaking near industrial/heavy trafficked sites. Heavy oil burning, ferrous/non-ferrous industry and vehicular emissions were identified as the main sources of atmospheric metal pollution.

A novel graphite furnace atomic absorption spectrometry (GFAAS) method was developed for refractory elements used as dopants in optical crystals. To overcome the crystal matrix induced effects (e.g. Bi_2TeO_5 and $LiNbO_3$), a regular graphite furnace heating program was extended with a halogenation cycle and liquid carbon tetrachloride was dispensed with a common GFAAS auto sampler. This method does not require any alteration to the graphite furnace gas supply system. The effectiveness of the method was verified with the determination of Er and Nd dopant elements in Bi_2TeO_5 crystals. A solid-sampling GFAAS method was elaborated for the determination of Mn in $LiNbO_3$ optical crystals based on the three-point-estimation standard addition techniques. The accuracy of the method was verified with the conventional, solution-based GFAAS method and by the solid-sampling analysis of a certified reference material.

The atomic absorption spectrometric (AAS) usability of the Electrolyte Cathode Atmospheric Glow Discharge (ELCAD) was studied with measuring aqueous standard solutions for Na, Cd, Zn and Cu. The ELCAD plasma was applied as the source of the atoms. The results showed that all these elements can be detected from the relatively low observation volume of the plasma of the ELCAD. The detection limits of AAS method for Na, Cd, Zn and Cu were determined and compared to that obtained from GFAAS.

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Grants and international cooperations

OTKA F 67647 Study on solid sampling spectrochemical methods for the analysis of optical crystals. (L. Bencs, 2007-10)

OTKA K 68390 Investigations of atomization processes in an electrolyte cathode atmospheric glow discharge. (P. Mezei, contributor L. Bencs, 2007-10)

OTKA CK 80896 Scintillator materials for medical imaging. (L. Kovács, contributors: Á. Péter, K. Polgár, G. Dravecz, 2010-13)

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HAS-Russian Academy of Sciences No. 18. Preparation and investigation of oxides with micro and nano-sized structures (K. Polgár, 2008-2010). Partner: A.V. Shubnikov Institute of Crystallography, RAS, Moscow.

HAS-Russian Academy of Sciences No. 23. Preparation and investigation of media for solid state lasers and stimulated Raman emission (K. Polgár, 2008-2010). Partner: General Physics Institute, RAS, Moscow.

HAS-Russian Academy of Sciences No. 22. Growth of single crystals with wide band-gap and investigation of their crystal lattice defects by spectroscopic methods (J. Janszky, K. Polgár, 2008-2010). Partner: Joffe Phys. Techn. Institute, RAS, St.Petersburg.

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See also: M.2., R.1., R.2., R.5., R.7.

R. CRYSTAL PHYSICS AND NONLINEAR OPTICS

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

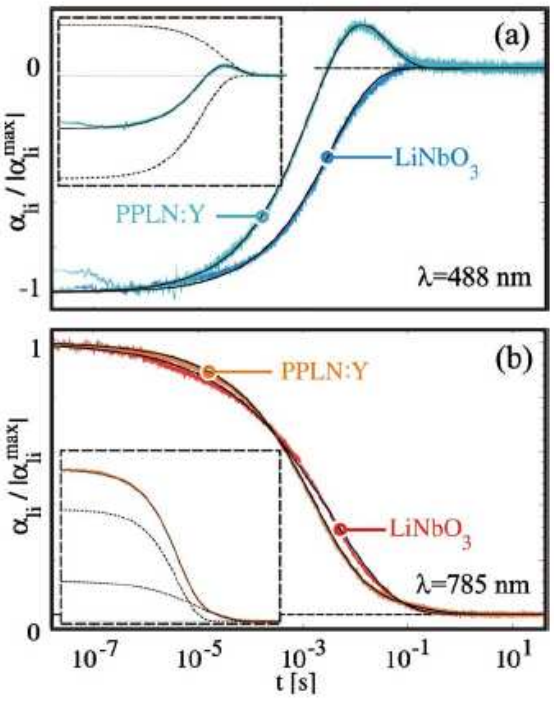

Fig. 1 *Temporal behavior of green laser-induced absorption in reduced periodically poled lithium niobate (PPLN:Y) and reduced single-domain nominally pure lithium niobate probed at (a) λ=488 nm and (b) λ=785 nm. Insets: complete fits for PPLN:Y (solid line) and its single components (dashed lines).*

Periodically poled $LiNbO_3$ single crystals monitored by transient absorption spectroscopy. — Laser-induced optical absorption transients were used to verify the non-uniform distribution of small polarons in thermochemically reduced periodically poled $LiNbO_3$:Y single crystals grown by the off-centre Czochralski method. The saw-tooth shaped distribution of the Y dopant in these crystals, accompanied by a similar but counter-phase distribution of Nb_{Li}^{5+} antisite defects, results upon reduction in a likewise periodic distribution of Nb_{Nb}^{4+}-Nb_{Li}^{4+} bipolarons, equivalent to bipolaronic layers with nearly unreduced layers in between. In one type of layer the green laser pulse induces a short-lived transparency in the green range by mainly destroying bipolarons while in the other type dominantly forming fresh electron and hole polarons yielding slightly more stable transient absorptions. The observed transients could be decomposed in the time domain without making spatially resolved measurements.

Nanohardness of double-doped $LiNbO_3$ single crystals. — Vickers nanoindentation experiments were carried out at loads between 0.1- 100 mN and at indentation depths from 10 up to 1150 nm on Z-cut samples polished in the same procedure using $LiNbO_3$ single crystals doped with 6 mol% Mg^{2+} and one of the following co-dopants: 1 mol% In^{3+}, 4 mol% Lu^{3+}, 1 mol% Gd^{3+} or 2 mol% Nd^{3+}. The obtained nanohardness values varied between 3.7 and 4.9 GPa and showed an increasing tendency with the increasing ionic radii of the second dopants.

Modelling of OH^- location and vibration in stoichiometric $LiNbO_3$. — Possible locations of protons incorporated in stoichiometric $LiNbO_3$ crystals were calculated using the SIESTA software code. The optimal, reduced-symmetry position of the H^+ ion was found next to a Li vacancy inside a triangle composed by oxygens having the longest O-O neighbor distance (d_{O-O}=3.36 Å) with an O-H bond near to a bisectrix and tilted at about 4.3 degrees out of the oxygen plane. The potential surface in a 1.2x1.2x1.2 $Å^3$ volume was evaluated and vibrational frequencies for the stretching and two bending modes were

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determined by both classical and quantum mechanical methods in agreement with the experiments.

Coherent radiative processes in rare earth doped $LiNbO_3$. — A simple, pulsed pump-probe measurement scheme has been worked out to measure the homogeneous linewidth of an atomic transition in an inhomogeneously broadened spectral line in a solid state environment. The theory was applied to the $^4I_{11/2} - {}^4I_{15/2}$ optical transition of erbium in $LiNbO_3:Er^{3+}$ crystal. By obtaining the homogeneous linewidth of (21.3 ± 0.4) MHz, a dipole relaxation time of about 90 ns has been determined. A population relaxation time of at about 2 ms has been estimated as well. Promising preliminary results have also been obtained for the case of the $^2F_{7/2} - {}^2F_{5/2}$ optical transition of ytterbium in $LiNbO_3:Yb^{3+}$ crystal.

Spectroscopy of Cu and Ag centres in lithium tetraborate single crystals. — In order to understand the properties of the tissue-equivalent thermoluminescent dosimeter and neutron detector material $Li_2B_4O_7$:Cu,Ag, the photoluminescence of Ag^+ centres has been separately characterized in single crystals of $Li_2B_4O_7$ single-doped with Ag and excited by synchrotron radiation at HASYLAB/DESY Germany. A single Ag^+ emission band was found at 4.6 eV, partly overlapping the previously investigated Cu^+ emission band at 3.35 eV, while the compound excitation spectrum of Ag^+ was identified in the 6-8 eV region also overlapping one of the corresponding excitation bands of Cu^+. Assignations of the underlying transitions of both ions involving d^{10} type ground and d^9s and/or d^9p type excited states are supported both by kinetic studies of the emission and theoretical modelling.

Design and fabrication of diffractive optical elements and waveguides by ion implantation. — Slab waveguides have been designed and fabricated in erbium-doped tellurite glass samples via implantation of 3.5 MeV N^+ ions at implanted doses of 1×10^{16} – 8×10^{16} ions/cm^2. Functionality tests (m-line spectroscopy) proved that all the waveguides worked. Waveguide operation at the 1550 nm telecommunication wavelength in this material has been demonstrated for the first time.

Beside glasses, slab optical waveguides were designed and fabricated in CaF_2, $Bi_4Ge_3O_{12}$ and $Bi_{12}GeO_{20}$ crystals, also using 3.5 MeV energy N^+ ions. Waveguides were characterised using UV/VIS and NIR absorption spectroscopy, spectroscopic ellipsometry and m-line spectroscopy. Implantation-induced absorption peaks, close to the UV absorption edge, were detected in both types of bismuth germanate crystals. First working slab waveguides fabricated in CaF_2 crystals using implantation of medium-mass ions in the MeV-energy range have been demonstrated. The waveguides implanted in birefringent bismuth germanate crystals were fully operative both in TE and TM mode up to 1550 nm.

Auger electron spectroscopy was used to determine depth distribution of implanted N^+ ions in thin films of silica (110 nm thick), grown on silicon substrates by chemical vapour deposition (CVD) and implanted by N^+ ions at an energy of 20 keV. The measurements revealed that implantation-induced refractive index modulation was sufficient for the production of efficient 10-layer Bragg gratings.

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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, 2006-2010)

OTKA K 68688 Fabrication of waveguides and diffractive optical elements via ion implantation (T. Lohner, HAS Research Institute for Technical Physics and Materials Science, contributors I. Bányász and A. Watterich, 2007 – 2010)

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

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)

HAS – Bulgarian Academy of Sciences joint project: Growth and spectroscopy of ferroelectric and multiferroic materials (L. Kovács, 2010-2012)

HAS – Polish Academy of Sciences joint project: Growth and spectroscopic investigation of rare-earth-doped nonlinear optical crystals (I. Földvári, contributors L. Kovács and K. Lengyel, 2008-2010)

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See also Q.4., Q.5., Q.8.

S. QUANTUM OPTICS AND QUANTUM INFORMATICS

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Cavity QED, Bose-Einstein condensates, many-body physics. — We have studied the dispersive optical bistability exhibited by a Bose-Einstein condensate of ultracold atoms inside the field of a laser-driven optical cavity by using a mean-field approximation and by analyzing the correlation functions of the linearized quantum fluctuations around the mean-field solution. The entanglement and the statistics of the atom-field quadratures have been given for the stationary state. We have shown that the mean-field solution, that is, the Bose-Einstein condensate, is robust against entanglement generation for most part of the phase diagram.

We showed that the motion of a laser-driven Bose-Einstein condensate in a high-finesse optical cavity realizes the spin-boson Dicke-model. The quantum phase transition of the Dicke-model from the normal to the superradiant phase corresponds to the self-organization of atoms from the homogeneous into a periodically patterned distribution above a critical driving strength. The fragility of the ground state due to photon measurement induced back action was calculated.

Quantum optics, laser-induced dynamics of atoms. — The fields in multiple-pass interferometers, such as the Fabry-Pérot cavity, exhibit great sensitivity not only to the presence but also to the motion of any scattering object within the optical path. We consider the general case of an interferometer comprising an arbitrary configuration of generic beam splitters and calculate the velocity-dependent radiation field and the light force exerted on a moving scatterer. We find that a simple configuration, in which the scatterer interacts with an optical resonator from which it is spatially separated, can enhance the optomechanical friction by several orders of magnitude.

We have described the propagation of a bichromatic light field in a resonant atomic medium using the Floquet-method. We have shown that new Raman-sidebands are generated in the course of propagation, and the generation of the modes is stable as long as adiabaticity is preserved for the atomic evolution.

Quantum information processing, quantum walks. — Quantum walks provide a useful tool to design efficient quantum algorithms. We analyzed the role of dimensionality in the time evolution of discrete-time quantum walks through the example of the three-state walk on a two-dimensional triangular lattice. The three-state Grover walk does not lead to trapping (localization) or recurrence to the origin, in sharp contrast to the Grover walk on the two-dimensional square lattice. We could prove that only a special subclass of coin operators can lead to recurrence and there are no coins that would lead to localization. The propagation for the recurrent subclass of coins is quasi-one dimensional.

We have proposed a definition for the Pólya number of continuous-time quantum walks to characterize their recurrence properties. We examined various graphs, including the ring, the line, higher-dimensional integer lattices, and a number of other graphs, we have calculated their Pólya number. For the timing of the measurements a Poisson process as well as regular timing were applied.

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Entanglement, spin squeezing. — We studied squeezing of the spin uncertainties by quantum non-demolition (QND) measurement in non-polarized spin ensembles. Unlike the case of polarized ensembles, the QND measurements can be performed with negligible back-action, which allows, in principle, perfect spin squeezing. The generated spin states approach many-body singlet states and contain a macroscopic number of entangled particles even when individual spin is large. We introduce the Gaussian treatment of unpolarized spin states and use it to estimate the achievable spin squeezing for realistic experimental parameters. Our proposal might have applications for magnetometry with a high spatial resolution or quantum memories storing information in decoherence free subspaces.

Highly polarized ensembles of identical spin-1/2 particles can be conveniently described by a single collective oscillator mode. We extended this model to general *d*-level atoms, and showed that such an ensemble is efficiently described by $d-1$ collective oscillators. Our theory provides better understanding of nonlinear light-matter interaction involving realistic multilevel atomic samples, and can be directly applied to atomic spin squeezing and ensemble quantum memories.

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Grants and international cooperations

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

OTKA NF68736 Cavity Quantum Electrodynamics of systems from few atoms to controlled ensembles (P. Domokos, 2007-2010)

TéT, Hungarian-Austrian Bilateral Intergovernmental S&T Cooperation (AT-3/2007): Quantized motion in an optical resonator (P. Domokos, 2008-2010)

TéT, Hungarian-Austrian Bilateral Intergovernmental S&T Cooperation (AT-2/2008): Decoherence effects in coherent quantum control processes in solids (Z. Kis, 2009-2010)

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.1. Adam P, Kiss T, Darázs Z, Jex* I; Conditional generation of optical Schrodinger cat states; *Phys Scr*; **T140**, 014011, 2010

S.2. Darázs Z, Kiss T; Pólya number of the continuous-time quantum walks; *Phys Rev A*; **81**, 062319/1-7, 2010

S.3. Földi* P, Kálmán O, Benedict* M G; Two-dimensional quantum rings with oscillating spin-orbit interaction strength: A wave function picture; *Phys Rev B*; **82**, 165322/1-8, 2010

S.4. Kollár B, Stefanák* M, Kiss T, Jex* I; Recurrences in three-state quantum walks on a plane; *Phys Rev A*; **82**, 012303/1-7, 2010

S.5. Kurucz Z, Mølmer* K; Multilevel Holstein–Primakoff approximation and its application to atomic spin squeezing and ensemble quantum memories; *Phys Rev A*; **81**, 032314/1-11, 2010

S.6. Nagy D, Domokos P, Vukics* A, Ritsch* H; Nonlinear quantum dynamics of two BEC modes dispersively coupled by an optical cavity; *Eur Phys J D*; **55**, 659–668, 2009

S.7. Nagy D, Konya G, Szirmai G, Domokos P; Dicke-model phase transition in the quantum motion of a Bose-Einstein condensate in an optical cavity; *Phys Rev Lett*; **104**, 130401/1-4, 2010

S.8. Ortigoso* J, Rodriguez* M, Santos* J, Kárpáti A, Szalay V; Long lasting molecular alignment: Fact or fiction?; *J Chem Phys*; **132**, 074105/1-13, 2010

S.9. Stefanák* M, Kollár B, Kiss T, Jex* I; Full revivals in 2D quantum walks; *Phys Scr*; **T140**, 014035, 2010

S.10. Szabó* L, Koniorczyk* M, Ádám P, Janszky J; Optimal universal asymmetric covariant quantum cloning circuits for qubit entanglement manipulation; *Phys Rev A*; **81**, 032323/1-6, 2010

S.11. Szirmai G, Nagy D, Domokos P; Quantum noise of a Bose-Einstein condensate in an optical cavity, correlations, and entanglement; *Phys Rev A*; **81**, 043639/1-14, 2010

S.12. Tóth G, Mitchell M.W*; Generation of macroscopic singlet states in atomic ensembles; *New J Phys*; **12**, 053007, 2010

S.13. Tóth G, Gühne O*; Separability criteria and entanglement witnesses for symmetric quantum states; *Appl Phys B*; **98**, 617, 2010

S.14. Urizar-Lanz I*, Tóth G; Number operator-annihilation operator uncertainty as an alternative of the number-phase uncertainty relation; *Phys Rev A*; **81**, 052108, 2010

S.15. Xuereb* A, Freegarde* T, Horak* P, Domokos P; Optomechanical Cooling with Generalized Interferometers; *Phys Rev Lett*; **105**, 013602/1-4, 2010

S.16. Xuereb* A, Freegarde* T, Horak* P, Domokos P; Scattering theory of multi-level atoms interacting with arbitrary radiation fields; *Phys Scr T*; **140**, 014010, 2010

S.17. Brougham* T, Kostak* V, Jex* I, Andersson* E, Kis* T; Entanglement preparation using symmetric multiports; *Eur Phys J D*; accepted for publication;

S.18. Z. Kis, S. Guérin, and H.R. Jauslin; Bichromatic field propagation in a resonant medium: Floquet analysis; *J Phys Conference Series;* accepted for publication

Conference proceeding

S.19. Wieczorek W*, Krischek R*, Ozawa A*, Tóth G, Kiesel N*, Michelberger P*, Udem T*, Weinfurter H*; Six-photon entangled Dicke state enabled by a UV enhancement cavity as novel SPDC photon source; Invited paper, keynote presentation in: *SPIE Photonics Europe, 12 - 16 April 2010, Brussels, Belgium*; Quantum Optics, edited by V.N. Zadkov, T. Durt, Proc. of SPIE **7727**; 77270L1-11, 2010

Others

S.20. Ádám P, Mechler* MI; Új fények a fizikában, Fizikus Vándorgyűlés, Pécs, 2010. augusztus 24-27 (New lights in Physics, Proceedings of the Physics Meeting, Pécs, Hungary); Eötvös Loránd Fizikai Társulat, Budapest, 2010; pp. 1-319, 2010

See also: R.3., R.4.

EDUCATION

Graduate and postgraduate courses, 2010

— Solid-state physics (J. Sólyom, ELTE[3])

— Electrons in solids (J. Sólyom, ELTE)

— Algebraic Bethe Ansatz and its application (F. Woynarovich, ELTE)

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

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

— Disordered systems (F. Iglói, SZTE)

— Many body systems II. (P. Szépfalusy and G. Szirmai, ELTE)

— Electronic states in solids (J. Kollár, ELTE)

— Superconductivity (I. Tüttő, ELTE)

— Advanced solid state physics I. (I. Tüttő, ELTE)

— Nanomagnetism (J. Balogh, ELTE)

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

— Amorphous and crystalline materials (S. Kugler* and T. Kemény, BME[5])

— Spectroscopy and material structure (K. Kamarás, BME)

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

— Macromolecules I. (S. Pekker ELTE)

— 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)

— Physics of granular materials (T. Unger* and T. Börzsönyi, BME)

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

— Superconductivity (G. Kriza, BME)

— Nanophase metals (I. Bakonyi, ELTE)

— Control theory (J. Füzi, PTE[6])

— Introduction to the neutron scattering for the microscopic investigation of matter, with applications in Physics, Chemistry, Biology and Geology (G. Nagy, Grenoble, France)

— Neutron beam methods in materials science, (L, Rosta, BME)

— Research of materials structures by neutron scattering (L. Rosta, ELTE)

[3] ELTE = Loránd Eötvös University, Budapest
[4] SZTE = University of Szeged
[5] BME = Budapest University of Technology and Economics
[6] PTE = University of Pécs

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

— From femtosecond lasers to attophysics (P. Dombi, SZTE)

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

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

— Mathematical methods in physics II. (P. Ádám, PTE)

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

— Open quantum systems (P. Ádám, PTE)

— Resonant light-matter interaction (P. Ádám, PTE)

— Quantum trajectory methods (P. Ádám, PTE)

— Vector calculus (P. Ádám, PTE)

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

— Quantum information by quantum optical means (T. Kiss, ELTE)

— Mechanics (P. Ádám, PTE)

— Mathematical methods in physics I., IV. (P. Ádám, PTE)

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

— Resonant light-matter interaction (P. Ádám, PTE)

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

— Laser cooling and trapping of atoms (P. Domokos, BME)

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

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

Laboratory practice and seminars

— Solid-state physics seminar (J. Sólyom, ELTE)

— Analysis (R. Juhász, PPKE[7])

— Seminar in quantum mechanics (B. Lazarovits, BME)

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

— Calorimetry (T. Kemény, 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, ELTE)

[7] PPKE = Pázmány Péter Catholic University

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

— Control theory practice (J. Füzi, PTE)

— Neutron detectors (J. Orbán, BME-INT[8])

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

— Practice course in introductory physics for computer engineers and informaticians (A. Szakál, BME)

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

— Medical application of lasers (Z. Gy. Horváth ; E-D Medical Laser Center)

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

— Spectroscopic investigation of OH in $LiNbO_3$ doped with damage resistant ions (K. Lengyel, BME)

Diploma works

F. Podmaniczky (BME): Density functional study of crystallization (Supervisor: T. Pusztai)

Á. Botos (ELTE): Preparation and characterization of carbon nanotubes filled with organic molecules

Zs. Kovács (ELTE, B.Sc.): Resonance phenomena during granular flow (Supervisor: T. Börzsönyi)

Sz. Kalácska (ELTE, B.Sc.): Fourier analysis of two-dimensional electroconvection patterns (Supervisor: N. Éber)

B. Szabó (ELTE, M.Sc.): Experimental investigations of layered granular materials under shear (Supervisor: T. Börzsönyi)

M. Dolgos (ELTE): Study of giant magnetoresistance (GMR) in Co/Cu multilayers (Supervisors: I. Bakonyi and L. Péter)

K. Szász (ELTE): Modelling the field dependence of magnetoresistance of GMR multilayers with various couplings and anisotropies (Supervisor: I. Bakonyi)

A. Sápi (ELTE): Study of the influence of high-energy heavy-ion irradiation and stress-annealing on the magnetic anisotropy of FINEMET materials by using Mössbauer spectroscopy (Supervisors: L.K. Varga (consulent) and E. Kuzmann[*])

F. Biró (ELTE): Preparation of iron coatings by non-stacionary electrochemical processes – Study of the microstructure and magnetic properties of the coatings (Supervisors: L.K. Varga (consulent) and M. Lakatos-Varsányi[*])

[8] Institute of Nuclear Techniques of the Budapest University of Technology and Economics

T. Verebélyi (ELTE): $Pd_{0.9}Ag_{0.1}H_x$ alloy; NMR study of a metallic hydrogen-storage model material (Supervisors: K. Tompa, M. Bokor and Gy. Bérces*)

O.K. Temesi (ELTE): Activation of Al-based alloys by liquid metals for hydrogen production via hydrolysis (Supervisor: L.K. Varga)

G. Gulyás (ELTE): Preparation and study of bulk amorphous and nanocrystalline alloys (Supervisor: L.K. Varga)

A. Szakál (BME): Atomic resolution holography measurements and evaluation (Supervisor: L. Cser)

B. Tóth (BME): Optimization of the working parameters of the mechanical neutron velocity selector (Supervisor: J. Füzi)

I. Márton (ELTE): Labview control of a time-of-flight spectrometer (Supervisors: P. Dombi, P. Rácz)

P. Heck (RheinAhrCampus, Remagen, Germany): Construction of a long-cavity Ti:sapphire oscillator (Supervisor: P. Dombi)

P. Sinkovicz (ELTE): Laser spectroscopy in single crystals doped with rare earth elements (Supervisors: Z. Kis and G. Mandula)

I. Kiss (BME): Thermal behaviour of hydroxyl ions in stoichiometric $LiNbO_3$ crystal (Supervisor: L. Kovács)

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 behavior 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 plaquatte ordering in interacting electron systems (Supervisor: K. Penc)

T.A. Tóth (EPFL[9]): Bilinear-biquadratic S=1 Heisenberg model on triangular and square lattices (Supervisors F. Mila* and K. Penc)

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

Zs. Szatmári (SZTE): Entaglement entropy of quantum spin chains (Supevisor: F. Iglói)

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

[9] Ecole Polytechnique Fédérale de Lausanne

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 (ELTE): Field theoretic description of far-from-equilibrium solidification morphologies (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)

É. Fazakas (ELTE): Preparation of bulk amorphous alloys by mechanical alloying (Supervisors: I. Bakonyi and L.K. Varga)

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)

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

A. Meiszterics (ELTE): Calcium containing bioceramics prepared by sol-gel method and their structure investigation (Supervisors: L. Rosta and K. Sinkó[*])

G. Nagy (ELTE, Université de Grenoble): Analysis of lamellar systems related to the photosynthesis with the use of neutron scattering (Supervisor: L. Rosta, J. Peters*, P. Timmins*, Gy. Garab*)

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

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)

V. Mile (ELTE): Diffraction and computer simulation studies of structural disorder in molecular liquids and solids (Supervisor: L. Pusztai)

P. Rácz (BME): (Supervisor: P. Dombi)

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

L. Vámos: Simulation models for aerosol characterization by elastic light scattering with special emphasis on photon correlation experiments in the nano-particle size range (Supervisor: P. Jani)

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)

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

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

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

L. Vitos: The Exact Muffin-Tin Orbitals method and applications. D.Sc.

G. Tegze (PhD, ELTE): Application of the phase-field crystal method to complex solidification processes (Supervisor: L. Gránásy)

Á. Pallinger (ELTE): Vortex dynamics in strongly anisotropic high-temperature superconductors (Supervisor: B. Sas)

J. Dégi (ELTE): Detailed study of mafic lower crustal xenoliths from the Bakony–Balaton Highland Volcanic Field — Relationships between metamorphic processes in the lower crust and the formation of the Pannonian Basin (Supervisors: Cs. Szabó* and K. Török*)

A. Len (PhD, ELTE): Tungsten wires studied by small angle neutron scattering (Supervisor: L. Rosta)

NK. Székely (PhD, ELTE): Small angle neutron scattering study on aqueous solutions of various diols and methylurea derivatives (Supervisor: L. Rosta)

Sz. Pothoczki (PhD, BME): Molekuláris folyadékok szerkezetének vizsgálata diffrakciós módszerekkel és számítógépes szimulációval (Structural studies of molecular liquids using diffraction methods and computer simulation methods, in Hungarian)

L. Vámos (PhD, BME): Simulation models for aerosol characterization by elastic light scattering with special emphasis on photon correlation experiments in the nano-particle size range (Supesvisor: P. Jani)

O. Kálmán (PhD, SZTE): Quantum interference in semiconductor rings (Supervisors M.G. Benedict* and P. Földi*)

D. Nagy (PhD, BME): Collective effects of radiatively interacting ultracold atoms in an optical resonator (Supevisor P. Domokos)

AWARDS

— V. Zólyomi: Talentum Award (Hungarian Academy of Sciences and the TALENTUM-CETA Foundation), 2009

— P. Dombi: International Gábor Dénes Award (Novoferr Foundation), 2009

— K. Kutasi: L'Oréal-UNESCO for Women in Science national award, 2010

— Z. Donkó: William Crooks Prize (European Physical Society & IOP Plasma Sources Science and Technology), 2010

— A. Czitrovszky: International Gábor Dénes Award (Novoferr Foundation), 2010

— G. Konczos: Knight's Cross, Order of Merit of the Hungarian Republic (civil division), 2010

— J. Füzi, SZFKI Applied Research Award, 2010

— P. Dombi, SZFKI Publication Award 2010

— T. Pusztai: Bolyai Grant (2007-2010)

— P. Jóvári: Bolyai Grant (2008-2011)

— P. Dombi: Bolyai Grant (2007-2010)

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

— K. Kutasi: Bolyai Grant (2008-2011)

— Z. Kis: Bolyai Grant (2007-2010)

— Z. Kis: APS Outstanding Referee

— P. Domokos: APS Outstanding Referee

MEMBERSHIPS

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
J. Kollár:	— Chairman of the Committee on Solid State Physics of the HAS
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 International Advisory Board, Condensed Matter Physics Conference
- Member of the Presidium of HAS
- Member of the Solid State Physics Committee of HAS

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)
- Member of the Editorial Advisory Board (2005-), Journal of Materials Science and Technology (Bulgaria, Sofia)
- Member of the Scientific Committee and Advisory Board (2nd Int. Conf. on Functional Nanocoatings, Dresden, 2010)
- 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-)
- 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 the Fellowship Board for Hungarian Science in the World, HAS (2008)

K. Tompa:
- Member of the Habilitation Committee of ELTE (2008-2010)
- 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

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:

— Member of ELI Participant Countries Council

— Head of the WG Optical Metrology in ELI

— President of the European Aerosol Assembly (EAA)

— 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 ELI Participant Council

— 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 Society 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

L. Bencs:

— Editorial Board member of Environmental Monitoring and Management (Internat. Journal)

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
J. Janszky:	— Member of the Editorial Board of Nonlinear and Quantum Optics
	— Member of the Editorial Board of Problems in Physics

CONFERENCES

— **Resonating Valence Bond Physics: Spin Liquids and Beyond**, Budapest, October 13-15, 2010, Organized by K. Penc, F. Mila, and A. Kiss. The workshop is dedicated to the memory of Patrik Fazekas, a former member of our institute. More than 35 participants attended the workshop from Europe, Japan, Canada and India.

— Second MAGFUM Swedish-Hungarian STINT workshop „**Magneto-mechanical properties of complex functional materials**", Budapest, November 11-12, 2010

— **EU FP7-Marie Curie Initial Training Network FINELUMEN**: midterm meeting, Sep 20-21, 2010, Katalin Kamarás, 20 participants

— **Microscopical and Spectroscopical Characterization of Multidimensional Materials (MISSA)**, joint workshop organized by the training networks PRAIRIES and FINELUMEN, Sep 22-23, 2010, organizer: Katalin Kamarás, 50 participants

— **EU FP6-Marie Curie Research Training Network PRAIRIES**: final meeting, Sep 24-25, 2010, organizer: Katalin Kamarás, 25 participants

— **Professional training in neutron research and instrumentation** was provided by the Neutron Spectroscopy Department (SZFKI), Nuclear Solid State Physics Department (RMKI) and the Mirrotron Co. for visiting scientists of the Institute of Nuclear Physics and Chemistry, Mianyang, China. The event has been held between July 10- August 26, 2010 at the MTA KFKI Research Campus in Budapest, consisting training in neutron scattering with specific orientation on neutron reflectometry, delivering lectures by leading scientists of the Budapest Neutron Centre (BNC) and hands-on-training using BNC neutron facilities.

— **The 5th Central European Training School on Neutron Scattering (CETS 2010)** has been held between May 31- June 04, 2010. The school was organized by the Neutron Spectroscopy Department and the Budapest Neutron Centre. The course provided an introduction to neutron scattering with special emphasis to hands-on-training at the BRR facilities. The training consisted of five days of tutorial lectures given by renowned lecturers from Europe including also major neutron centers like Dubna, FRM II, HZ-Berlin, ILL.

— **Neutron source spallation target workshop** has been held on the 2nd July 2010 at the KFKI campus co-hosted by the Atomic Energy Research Institute, HAS and the Research Institute for Solid State Physics and Optics, HAS, with the participation of Mirrotron Co., the Japan Proton Accelerator Research Complex (JPARC) and the Rogante Engineering Office (Italy). Lectures were focused on spallation neutron source development, considering different target options and industrial aspects of some target related issues.

— **XXXI European Conference on Laser Interaction with Matter**, Budapest, 6-10 September 2010, organizers: I. Földes*, P. Dombi. The conference, traditionally started as a yearly meeting of the laser fusion community in Europe, attracted more than 140 participants from all over the continent, Japan and USA. This year the topics were extended with attophysics and laser particle acceleration and a special session was devoted to research activities related to the ELI project (Extreme Light Infrastructure).

— **11th Europhysical Conference on Defects in Insulating Materials (EURODIM 2010)**, Pécs, 12-16 July 2010, organised by L. Kovács, more than 200 participants from 31 countries in Europe, Asia, Africa and the Americas. The topic covered the research and technology of defect-related phenomena in crystalline and amorphous wide band-gap bulk, layered and nano-materials. The papers will be published in IOP Conference Series: Materials Research and Engineering.

TABLE OF CONTENTS