ANNUAL REPORT

2009

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

Research Institute for Solid State Physics and Optics

Hungarian Academy of Sciences

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ANNUAL REPORT 2009

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 16th 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. Application oriented research and development focuses on optical thin films, laser applications, growth of optical crystals, and metallurgy.

Our institute is actively participating in several projects within the EU 7th Framework Programme. The success story of this year is winning the site choice competition within the Extreme Light Infrastructure (ELI), an ESFRI project, together with the Czech Republic and Romania. The Hungarian participation in the ELI-PP project is coordinated by our institute.

Our staff of 189 includes 124 scientists. This year we have published more than 200 papers in high quality international journals and conference proceedings showing a steadily high publication activity over the last years. The textbook "Fundamentals of the Physics of Solids, I. Structure and Dynamics" by Jenő Sólyom was published in Hungarian this year.

The achievements of our scientists have been acknowledged by several awards and nominations. Norbert Kroó has received the Willis E. Lamb Award for Laser Science and Quantum Optics, and was nominated as Honorary Doctor at the ELTE University. Örs Legeza received the DSc title at the Hungarian Academy of Sciences. Seven of our young researchers have received their PhD degree.

It has become a tradition of the institute to deliver prizes for outstanding publication activity. In 2009 the Publication Prize has been won by Róbert Juhász for his papers published on the theoretical studies of different aspects of equilibrium and non-equilibrium statistical physics.

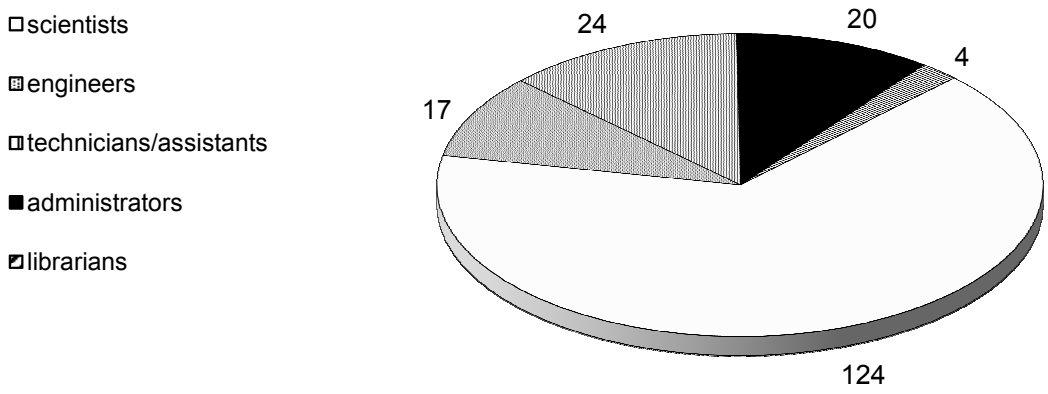
I hope this booklet will provide you with useful information. The key figures offer a general overview of our institute as a whole. In order to facilitate the access to our scientists, we included their direct e-mail addresses in the Annual Report for your convenience. For further information please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

Budapest, December 4, 2009.

János Kollár
Director

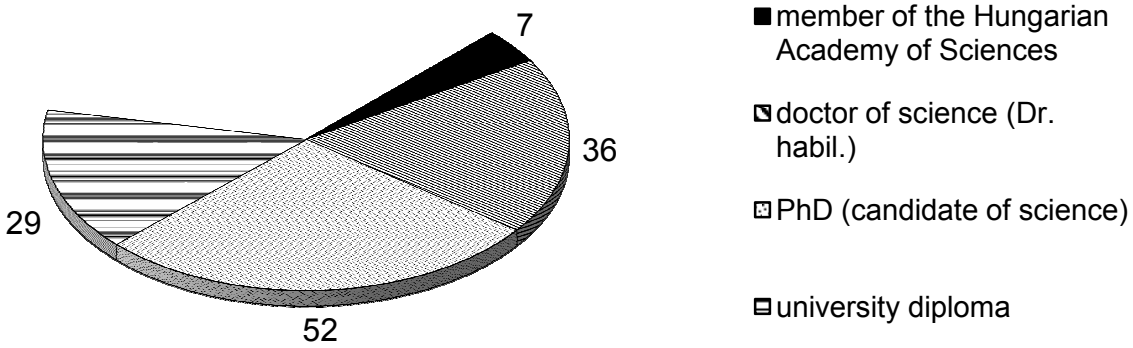
KEY FIGURES

Permanent staff of the institute: 189 employees. Its distribution by professions:

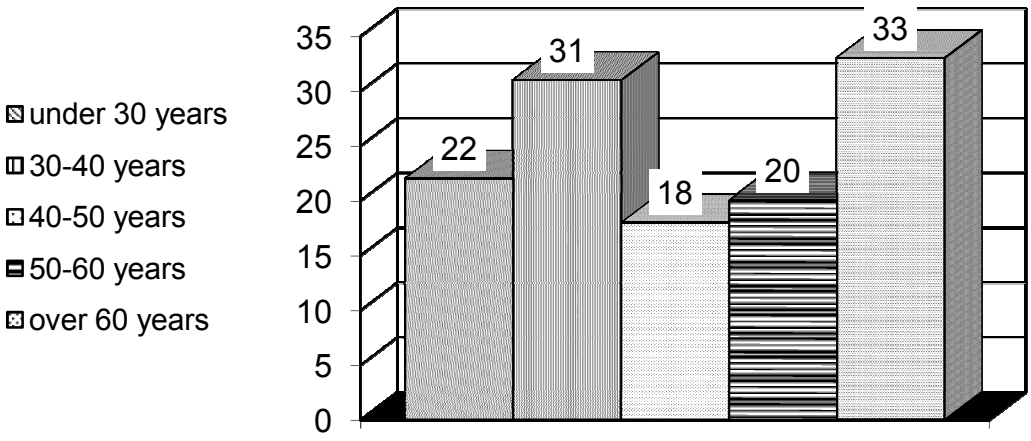


Distribution of scientists:

a) by scientific titles/degrees:

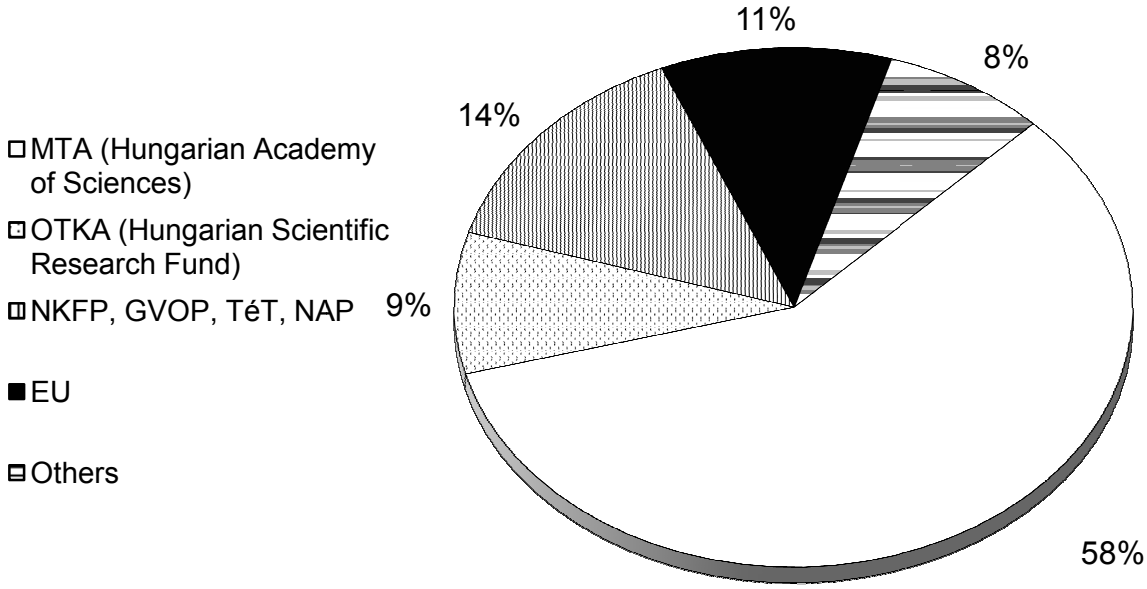


b) by age groups:

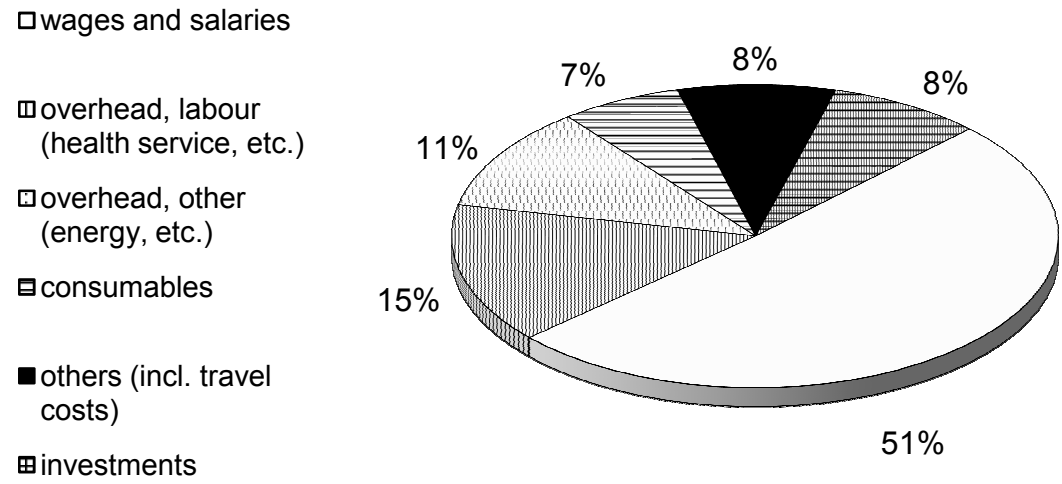


Financial management

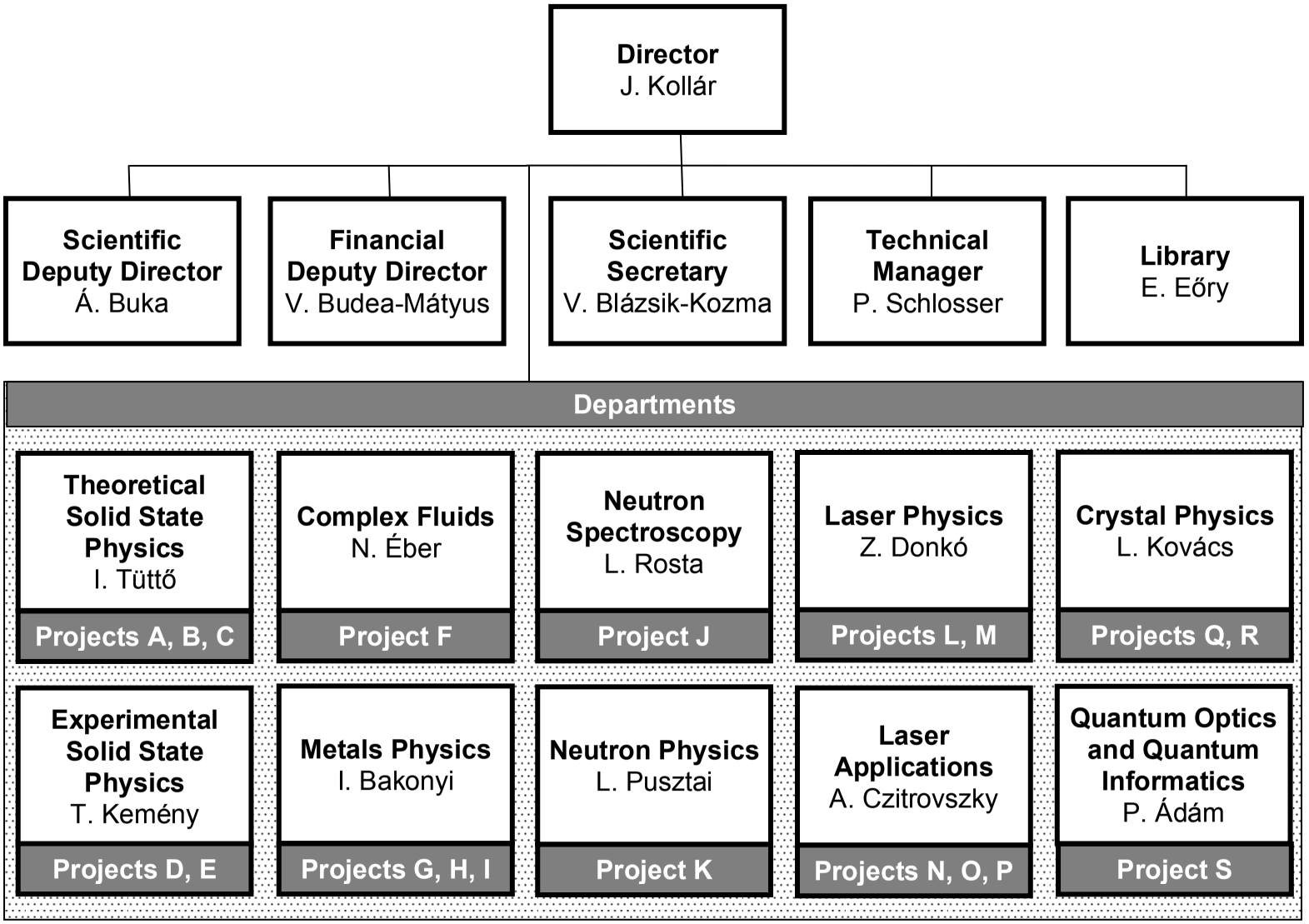
a) Sources of operation costs:



b) Distribution of expenditures:



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



A. STRONGLY CORRELATED SYSTEMS

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

Low-dimensional fermionic models. — We have continued the study of quantum phase transitions by using the density-matrix renormalization-group (DMRG) method. We examined the phase diagram of the half-filled one-dimensional extended Hubbard model using quantum information entropies. A charge-density-wave phase is known to exist for weak on-site and strong nearest-neighbor Coloumb repulsion. The ground state is a spin-density wave for strong on-site and weak nearest-neighbor Coloumb repulsion. An additional new, bond-order phase has been found between them in a narrow range of couplings. The transition from the charge-density-wave phase changes from first order to second order in the parameter regime where all three phases are present. We presented evidence that the transition between the spin-density-wave and bond-order phases is of infinite order.

In order to understand the magnetic properties of the 1D non-half-filled attractive Hubbard model we analyzed both analytically and numerically the behavior of the energy near the critical field. We have demonstrated that the extremely high but nondivergent susceptibility is caused by a collective effect: the breaking up of bound pairs to produce magnetic excitations changes the distribution of the pairs.

We have also studied the elementary excitations of a model Hamiltonian for the π-electrons in poly-diacetylene chains, where the bare band gap is only half of the single-particle gap and the binding energy of excitons (0.5 eV) amounts to 20% of the single-particle gap. Employing both the Hubbard−Ohno potential and the screened potential, we have reproduced the experimental results for the binding energy of the singlet exciton and its polarizability. Our results have indicated that there are optically dark states below the singlet exciton, in agreement with experiment. In addition, we have found a weakly bound second exciton with a binding energy of 0.1 eV.

Coexistence of superconductivity and density waves. — Superconductivity seems to compete with spatially nonuniform magnetic order in high-temperature superconductors. In an “exotic” phase of matter, the so-called supersolid, superfluidity and nonuniform spatial order are simultaneous present. We investigated the coexistence and competition of density waves and pairing in a fermion model with nesting Fermi surface within a BCS-like mean-field treatment. In addition to the usual zero-momentum Cooper pairs, the formation of nonzero-momentum pairs is also allowed for. We found that the two types of ordering may coexist in the ground state, and momentum-dependent superconductivity occurs due to the presence of the inhomogeneous charge order. The momentum of the Cooper pairs is identical to that of the density wave.

A quantum liquid with deconfined fractional excitations in three dimensions. — Excitations which carry "fractional" quantum numbers are known to exist in one and two dimensions. Fractional excitations have also been invoked to explain the breakdown of the conventional theory of metals in a wide range of three-dimensional materials. Their existence remains, however, highly controversial. Using Green's function Monte-Carlo method and perturbation theory, we have found direct numerical evidence for the existence of a quantum liquid phase supporting fractional excitations in a three-dimensional

[#] PhD student

microscopic model − the quantum dimer model on a diamond lattice. We demonstrated explicitly that the energy cost of separating fractional monomer excitations vanishes in this liquid phase, and that its energy spectrum matches that of the Coulomb phase in (3+1) dimensional quantum electrodynamics.

Bond-wave calculation of the ESR spectra in $SrCu_2(BO_3)_2$. — $SrCu_2(BO_3)_2$ is a spin-gap system constituted of orthogonal dimers of Cu ions. We are interested in the role of Dzyaloshinskii-Moriya (DM) interaction that is inherently present in this material. Starting from a bond factorized wave function, we have mapped out the variational phase diagram for low magnetic field and finite DM interactions, including the symmetry analysis of the different phases. Using bosons to describe the states of a two spin-1/2 dimer, we extended the usual spin-wave theory to get the magnetic-field evolution of the ESR spectra for different cases of the DM interactions, and compared it to the ESR measurements.

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Grants

OTKA[1] K62280	Phase transitions in correlated electron systems: Theory and NMR experiments (P. Fazekas, now K. Penc, 2006-2009)
OTKA 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)

Publications

Articles

A.1. Tóth* AI, Moca* CP, Legeza Ö, Zaránd* G; Density matrix numerical renormalization group for non-Abelian symmetries; *Phys Rev B*; **78**, 245109/1-11, 2008

A.2. Mund* C, Legeza Ö, Noack* RM; Quantum information analysis of the phase diagram of the half-filled extended Hubbard model; *Phys Rev B*; **79**, 245130/1-7, 2009

A.3. Lante* V, Rousochatzakis* I, Penc K, Waldmann* O, Mila* F; Field-induced magnetoelastic instabilities at level crossings in antiferromagnetic molecular wheels; *Phys. Rev. B*; **79**, 180412/1-4, 2009

[1] OTKA: Hungarian Scientific Research Fund

A.4. Barcza G, Legeza Ö, Gebhard* F, Noack* RM; Density-matrix renormalization-group study of excitons in poly-diacetylene chains; arXiv:0908.4160, accepted for publication

A.5. Sikora* O, Pollmann* F, Shannon* N, Penc K, Fulde* P; Quantum liquid with delocalized fractional excitations in three dimensions; *Phys Rev Lett*; accepted for publication

Conference proceedings

A.6. Szirmai E, Legeza Ö, Sólyom J; The role of the exchange interaction in the one-dimensional *n*-component Hubbard model; In: *Proceedings of the European Conference "Physics of Magnetism 08" Poznan 2008, Acta Physica Polonica A;* **115**, 98-100, 2009

A.7. 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*, accepted for publication

Book

A.8. Sólyom J; A modern szilárdtest-fizika alapjai. I. Szerkezet és dinamika (Fundamentals of the Physics of Solids, I. Structure and Dynamics, in Hungarian), Eötvös Kiadó, 2009

Others

A.9. Szirmai E; Egydimenziós világ - gyakorlati haszon, Csőbe húzott elektronok (One-dimensional world - practical use, in Hungarian); *Élet és Tudomány*; **29**, 909-911, 2009

A.10. Woynarovich F; A Középiskolai Matematikai és Fizikai Lapok Fizika Rovata (The Physics Section of the Mathematical and Physical Journal for Secondary Schools, in Hungarian) Proc. of the seminar *Fizika Tanítás Tartalmasan és Érdekesen*, 2009; Ed: PhD School in Physics of the Roland Eötvös University

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. — We have considered the critical behavior of the random q-state Potts model in the large-q limit with different types of disorder leading to either the nonfrustrated random ferromagnet regime (with a parameter $p > 0$) or the frustrated spin-glass regime ($p < 0$). The model is studied on the diamond hierarchical lattice for which the Migdal-Kadanoff real-space renormalization is exact. It is shown to have a ferromagnetic and a paramagnetic phase and the phase transition is controlled by four different fixed points. The state of the system is characterized by the distribution of the interface free energy $P(I)$ which is shown to satisfy different integral equations at the fixed points. By numerical integration we have obtained the corresponding stable laws of nonlinear combination of random numbers and obtained numerically exact values for the critical exponents (Fig.1).

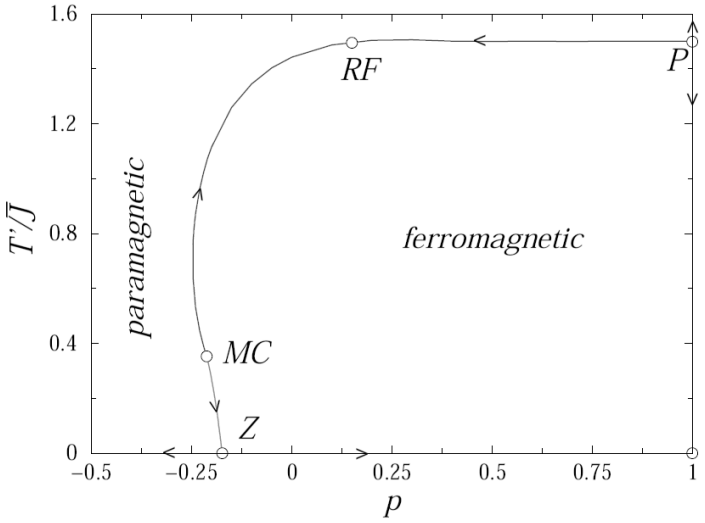

Fig.1 *Phase diagram of the disordered Potts model as a function of temperature T' and frustration parameter p.*

We have considered two fully frustrated Ising models: the antiferromagnetic triangular model in a field of strength, $h = HTk_B$, as well as the Villain model on the square lattice. After a quench from a disordered initial state to $T = 0$ we studied the nonequilibrium dynamics of both models by Monte Carlo simulations. In a finite system of linear size, L, we defined and measured sample dependent "first passage time", t_r, which is the number of Monte Carlo steps until the energy is relaxed to the ground-state value. The distribution of t_r, in particular its mean value, $\langle t_r(L)\rangle$, is shown to obey the scaling relation, $\langle t_r(L)\rangle \sim L^2 \ln(L/L_0)$, for both models. Scaling of the autocorrelation function of the antiferromagnetic triangular model is shown to involve logarithmic corrections, both at $H = 0$ and at the field-induced Kosterlitz-Thouless transition, however the autocorrelation exponent is found to be H dependent.

We have studied a coagulation process, which is controlled by a parameter $\omega \in [-1,1]$ and interpolates between known statistical physical models: The case $\omega = -1$ corresponds to the strong disorder renormalisation group transformation of certain disordered quantum spin chains whereas $\omega = 1$ describes coarsening in the one-dimensional Glauber-Ising model. The case $\omega = 0$ is related to the renormalisation group transformation of a recently introduced graph with a fat-tail edge-length distribution. In the intermediate range $-1 < \omega < 1$, the exponents α_ω and β_ω that characterise the growth of the primary and secondary variable, respectively, are accurately estimated by analysing the differential equations

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describing the process in the continuum formulation. According to the results, the exponent α_ω varies monotonically with ω while β_ω has a maximum at $\omega = 0$.

We have investigated with numerical methods the phase diagram of a one-dimensional model with three absorbing phases (generalized Hinrichsen model) and found, in some relatively narrow range of the parameter space of the model a sequence of critical behaviors from absorbing to active phases with non-universal exponents. The final conclusions are still under consideration and further computer studies are under way.

Quantum systems. — The quantum Ising chain of length, L, which is separated into two parts by localized or extended defects has been considered at the critical point where scaling of the interface magnetization is non-universal. We have measured the entanglement entropy between the two halves of the system in equilibrium, as well as after a quench, when the interaction at the interface is changed for time $t > 0$. For the localized defect the increase of the entropy with $\log L$ or with $\log t$ is found to involve the same effective central charge, which is a continuous function of the strength of the defect. On the contrary for the extended defect the equilibrium entropy is saturated, but the non-equilibrium entropy has a logarithmic time-dependence the prefactor of which depends on the strength of the defect.

We have studied 3 fluid hydrodynamics in gases with spin-1 Bose-Einstein condensates in the P2 polar phase. The velocities of the hydrodynamic modes have been determined as a function of the temperature and the applied magnetic field. The critical mode has been identified near the transition to the other polar phase (P1).

We studied the possibility of coexistence of diagonal and off-diagonal long-range orders in certain models of bosons. According to an old suggestion by Russian physicists, integrable pair potentials with a partly negative Fourier transform may have such a "coherent crystal" ground state at sufficiently high densities. While the original suggestion was based on Hartree approximation, we proved this property for a periodic mean-field type interaction.

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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)
MTA-DFG/193	Statistical physics of disordered systems (F. Iglói, 2008-2009)

Publications

Articles

B.1. Karsai* M, Kovács IA, Anglès d'Auriac* J-Ch, Iglói F; Density of critical clusters in strips of strongly disordered systems; *Phys Rev E;* **78**, 061109/1-9, 2008

B.2. Eisler* V, Iglói F, Peschel* I; Entanglement in spin chains with gradients; *J Stat Mech*; P02011/1-17, 2009

B.3. Iglói F, Szatmári* Zs, Lin* Y-C; Entanglement entropy with localized and extended interface defects; *Phys Rev B;* **80**, 024405/1-9, 2009

B.4. Karsai* M, Anglès d'Auriac* J-Ch, Iglói F; Nonequilibrium dynamics of fully frustrated Ising models at T=0; *J Stat Mech*; P07044/1-14, 2009

B.5. Iglói F, Turban* L; Disordered Potts model on the diamond hierarchical lattice: Numerically exact treatment in the large-q limit; *Phys Rev B;* **80**, 134201/1-9, 2009

B.6. Juhász R; Superdiffusion in a class of networks with marginal long-range connections; *Phys Rev E*;**78**, 066106/1-9, 2008

B.7. Juhász R; A non-conserving coagulation model with extremal dynamics; *J Stat Mech*; P03033/1-14, 2009

B.8. Juhász R, Ódor* G; Scaling behavior of the contact process in networks with long-range connections; *Phys Rev E;* **80**, 041123/1-8, 2009

B.9. Sütő A; A possible mechanism of concurring diagonal and off-diagonal long-range order for soft interactions; *J Math Phys*; **50**, 032107/1-12, 2009

C. ELECTRONIC STATES IN SOLIDS

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

Using the density functional theory, we present a systematic theoretical study of the **layer relaxation** and **surface stress** of 5d transition metals. Our calculations predict layer contractions for all surfaces, except for the (111) surface of face centered cubic Pt and Au, where slight expansions are obtained similarly to the case of the 4d series. We also find that the relaxations of the close packed surfaces decrease with increasing occupation number through the 5d series. The surface stress for the relaxed, most closely packed surfaces shows similar atomic number dependence as the surface energy. Using Cammarata's model and our calculated surface stress and surface energy values, we examine the possibility of surface reconstructions, which is in reasonable agreement with the experimental observations.

Duplex stainless steels have many superior properties compared to conventional steels, this being mainly due to their microstructure containing approximately equal amount of ferrite and austenite phases formed by iron, chromium (or Cr equivalent), and nickel (or Ni equivalent). Using computational methods based on first-principles theories, the phase stability of paramagnetic $Fe_{1-c-n}Cr_cNi_n$ alloys ($0.12<c<0.32$ and $0.04<n<0.32$) at high temperatures (>1000 K) is addressed. It is shown that the stabilization of the ferrite-austenite two-phase field in duplex steels is a result of complex interplay of several competing phenomena. Taking into account only the formation energies yields a complete phase separation, strongly overestimating the two-phase region. The formation energies are calculated to be lower for the austenite than for the ferrite, meaning that the configurational entropy has a more significant impact on the stability field of the austenitic phase. The magnetic and vibrational free energies have opposite effects on the phase stability. Namely, the magnetic entropy favors the ferrite phase, whereas the vibrational free energy stabilizes the austenite phase. Combining the formation energies with the magnetic, vibrational, and configurational free energies, a region of coexistence between the two phases is obtained, in line with former thermodynamic assessments as well as with experimental observations.

The composition and the structure of the **Earth's solid inner core** are still unknown. Iron is accepted to be the main component of the core. Lately, the body-centered cubic (bcc) phase of iron was suggested to be present in the inner core, although its stability at core conditions is still in discussion. The higher density of pure iron compared with that of the Earth's core indicates the presence of light element(s) in this region, which could be responsible for the stability of the bcc phase. However, so far, none of the proposed composition models were in full agreement with seismic observations. The solubility of magnesium in hexagonal Fe has been found to increase significantly with increasing pressure, suggesting that Mg can also be an important element in the core. Here, we report a first-principles density functional study of bcc Fe–Mg alloys at core pressures and temperatures. We show that at core conditions, 5–10 atomic percent Mg stabilizes the bcc Fe both dynamically and thermodynamically. Our calculated density, elastic moduli, and sound velocities of bcc Fe–Mg alloys are consistent with those obtained from seismology,

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indicating that the bcc-structured Fe–Mg alloy is a possible model for the Earth's inner core.

Ab initio total-energy calculations, based on the exact muffin-tin orbital method, are used to determine the elastic properties of **$Pd_{1-x}Ag_x$ random alloys** in the face-centered-cubic crystallographic phase. The compositional disorder is treated within the coherent-potential approximation. The single crystal and polycrystalline elastic constants and the Debye temperature are calculated for the whole range of concentration, $0<x<1$. It is shown that the variation in the elastic parameters of Pd-Ag alloys with chemical composition strongly deviates from a simple linear or parabolic trend. The complex electronic origin of these anomalies is demonstrated.

The single-crystal and polycrystalline **elastic constants** and the elastic anisotropy in face-centered cubic and hexagonal close-packed **FeNi alloys** have been investigated at ultrahigh pressures by means of first-principles calculations using the exact muffin-tin orbitals method and the coherent-potential approximation. Comparisons with earlier calculations for pure Fe and experimental results are presented and discussed. We show that Ni alloying into Fe increases slightly the density and has very little effect on bulk moduli. Moreover, the relative decrease in c_{44} elastic constant is much stronger in the hcp phase than in the fcc one. It is found that the elastic anisotropy is higher for face-centered cubic than for the hexagonal close-packed structure of FeNi, even though the face-centered cubic phase has a higher degree of symmetry. The anisotropy in face-centered cubic structure decreases with increasing nickel concentration while a very weak increase is observed for the hexagonal close-packed structure.

Using the ab initio exact muffin-tin orbitals method in combination with the coherent-potential approximation, we have calculated the **elastic parameters** of ferromagnetic $Fe_{1-m}Mg_m$ ($0<m<0.1$) and $Fe_{1-c}Cr_c$ ($0<c<0.2$) **random alloys** in the body-centered cubic (bcc) crystallographic phase. Results obtained for $Fe_{1-c}Cr_c$ demonstrate that the employed theoretical approach accurately describes the experimentally observed composition dependence of the polycrystalline elastic moduli of Fe-rich alloys encompassing maximum 10% Cr. The elastic parameters of Fe-Cr alloys are found to exhibit anomalous composition dependence around 5% Cr. The immiscibility between Fe and Mg at ambient conditions is well reproduced by the present theory. The calculated lattice parameter for the Fe-Mg regular solid solution increases by 1.95% when 10% Mg is introduced in Fe, which corresponds approximately to 11% decrease in the average alloy density, in perfect agreement with the experimental finding. At the same time, we find that all of the elastic parameters of bcc Fe-Mg alloys decrease almost linearly with increasing Mg content. The present results show a much stronger alloying effect for Mg on the elastic properties of α-Fe than that for Cr. Our results call for further experimental studies on the mechanical properties of the Fe-Mg system.

We have performed first principles density functional theory studies of various **carbon nanostructures**. In particular we performed calculations on the phonon dispersion of single walled carbon nanotubes in the helical Brillouin zone which is invaluable for the interpretation of Raman experiments. We also studied junctions of different types of nanotubes, looking at the localized states which appear at the junction. In relation the Luttinger liquid behavior and the weak ESR signal of carbon nanotubes, we also studied the electronic density of states. Finally, we performed calculations on doped fullerene-cubane cocrystals with a two-component doping which provides triple negative fullerene ions in the cocrystal.

We investigated the **surface Rashba effect** subject to reduced in-plane symmetry. Based on a *K.p* perturbation theory, we derived a detailed microscopic description of the Anisotropic Rashba Splitting (ARS). Furthermore, we show that this ARS can not be explained within the standard theoretical picture of the Rashba effect assuming a purely normal-to-surface variation of the crystal potential. The new microscopic expression for the Rashba Hamiltonian is explicitelly supported by fully relativistic first principles calculations for Fe and Co impurities on (100), (110) and (111) surfaces of Cu, Au and Pt. We showed that there is at least three different mechanism for the impurities to interact. On the (111) and (110) surfaces, where there is surface state, the frequency of oscillation depends on the Fermi vector of the surface state, while on (100) surface where the surface state is above the Fermi level, there is no long-range oscillation. On the Au(111) surface due to the large spin orbit coupling, the interaction oscillates with two frequencies, in perfect agreement of the Rashba splitting of the surface state. We studied the nature of the interaction in the deeper layers as well.

We continued our work to describe the **non-equilibrium properties of quantum dots**. A quantum dot with even number of electrons was studied close to the singlet-triplet transition considering a two level Anderson model. A wide range of the parameters was considered in order to explore the limitations of the applied theoretical method, the iterative perturbation theory. In order to study the electronic structure of vanadium-dioxide we performed cluster-DMFT (CTQMC) calculations both in its low- (M1) and high-temperature (rutile) phases. Motivated by the recent efforts directed towards tuning the **physical properties of vanadium-dioxide** by depositing films on different supporting surfaces of different orientations we performed calculations for different geometries for both phases. Our main focus was to identify the mechanisms governing the formation of the gap characterizing the M1 phase and its dependence on the geometry. We found that the increase of the band-width with compression along the axis corresponding to the rutile c-axis is more important than the so-called Peierls bonding-antibonding splitting which is usually believed to be the most important mechanism in the gap formation.

Since there is mounting evidence that the pseudogap phase of underdoped **high-T_c superconductors** is an **unconventional density wave** (UDW), we have investigated theoretically the optical and Raman response of cuprates in the region of their phase diagram, where the superconducting and UDW order parameters compete and coexist. Our most interesting finding is that contrary to conventional wisdom, the UDW condensate does contribute to the Raman intensity, at least in the A_{1g} and B_{1g} symmetries. In addition, we have summarized our results on the Landau quantization of the Dirac spectrum of quasiparticles in UDW. Careful analysis of the angular dependent magnetoresistance and Nernst effect data shows that in certain parts of their phase diagram, UDW is the ground state of a number of materials including organic charge transfer salts and cuprate superconductors.

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Grants and international cooperations

OTKA T048827 First principles calculations for surfaces; surface stress and segregation (J. Kollár, 2005-2009)
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)

Publications

Articles

C.1. Zólyomi V, Kollár J, Vitos L; Anomalous surface relaxation in hcp transition metals; *Phys Rev B*; **78**, 195414/1-5, 2008

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See also: H.1.

D. NON-EQUILIBRIUM ALLOYS

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

Pressure dependent magnetic properties. — Research of pressure dependent magnetoelastic properties of Fe-based amorphous alloys is in the limelight since it revealed the fundamental relation between the volume stability of Fe-moment and features of the electronic structure of Fe-based materials. Recently, the Fe-based amorphous alloys have been applied as starting materials for the preparation of useful nanostructures. The hydrostatic pressure changes the average atomic volume and consequently influences the intrinsic magnetic properties of these alloys, e.g. Curie temperature (T_C) and saturation magnetic moment. The installation of a pressure cell inside the SQUID magnetometer at the end of last year – after the necessary test measurements – made us capable to study the pressure dependence of the magnetic properties.

For methodical reasons amorphous $Fe_{56}Mn_{24}B_{20}$ and $Fe_{60}Mn_{20}B_{20}$ alloys with relatively low Curie points were chosen to be studied. Both amorphous Fe-Mn-B alloys show two characteristic magnetic transitions at ambient pressure: (1) the paramagnetic (PM) - ferromagnetic (FM) transition at the Curie temperature T_C = 202 and 163 K and (2) a spin freezing transition at temperature T_f = 8.5 and 13 K, respectively. The Curie point is defined as the inflection point of $M(T)$ curves measured in 10 Oe magnetic field. T_C decreases with increasing pressure, as it is illustrated in Fig. 1 for the 20 at% Mn alloy, dT_C/dp = -3.3 and -2.3 K/kbar for the 20 and 24 at% Mn alloys, respectively.

Fig. 2 shows the magnetization measured in a magnetic field of 5 T for $Fe_{60}Mn_{20}B_{20}$ as a function of temperature at different pressures. Similar curves were obtained for the alloy with 24 at% Mn content. The saturation magnetization at low temperature, M_0, shows a remarkable decrease with increasing pressure, $d\ln M_0/dp$ = -0.016 and -0.009 $kbar^{-1}$ for the 20 and 24 at% Mn alloys, respectively. An apparent increase of M_0 can be observed with increasing pressure from the ambient to the first high-pressure value at low temperature. This apparent increase is of methodological origin related with the freezing of the pressure transmitting medium. This way, the values determined at p = 1 bar was not considered in the calculation of the pressure derivatives of M_0.

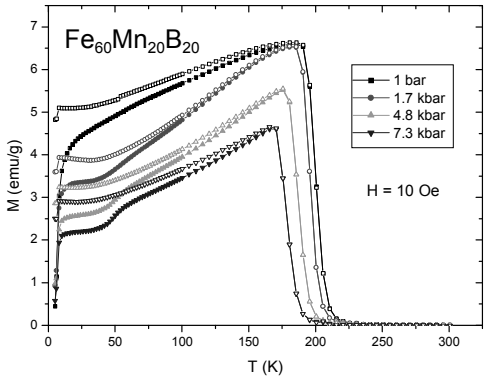

Fig. 1 *Temperature dependence of magnetization for $Fe_{60}Mn_{20}B_{20}$ measured in a magnetic field of 10 Oe after zero-field cooling (ZFC, full symbols) and field cooling in 10 Oe (FC, open symbols) at different pressures indicated.*

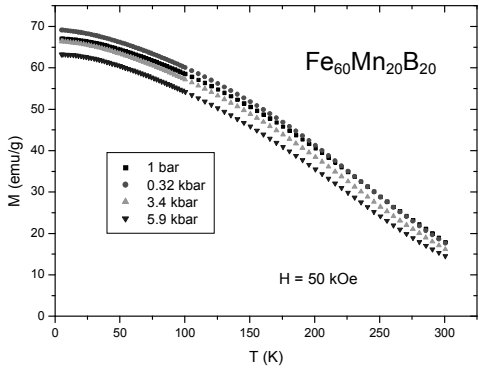

Fig. 2 *Magnetization measured in 5 T for $Fe_{60}Mn_{20}B_{20}$ as a function of temperature at different pressures.*

The observed effect of pressure on the Curie temperature and the saturation magnetization is rather large for both amorphous alloys studied. The decrease of the saturation magnetization is one order of magnitude larger than that expected from theoretical calculations for amorphous iron and amorphous Fe-B alloys.

Magnetic properties of Fe-Ag granular alloys and discontinuous multilayers. — Fe-Ag co-deposited granular alloy and discontinuous multilayer samples with 10-36 at% Fe average compositions were prepared by vacuum evaporation onto Si(111) single crystal substrates at room temperature. The magnetic properties of the samples were studied by SQUID and in-field Mössbauer spectroscopy. Superparamagnetic behavior was observed for all the samples with blocking temperatures (T_B) steeply increasing with increasing Fe concentration. Two significant differences were observed between the different sample sets: the temperature dependence of the 5T magnetization and the appearance of perpendicular anisotropy. The bulk magnetization (M) measured in 5 T shows linear temperature dependence for both series but the relative decrease of M with temperature is much larger for a granular alloy than for a multilayer sample of equal T_B. It is explained by the larger amount of non-aligned small grains in the co-evaporated alloy. For ultra small Fe layer thickness a perpendicular anisotropy appears in the multilayer samples, which can also be observed as a different shape of the magnetization curve of the $Fe_{10}Ag_{90}$ sample pair and thereby influencing the grain size obtained from a Langevin fit to the bulk magnetization data. When the simple large-field approximation ($M(H) \sim M(\infty)$ (1 - $kT/\mu H$)) is used in the evaluation, the average grain size obtained for the $Fe_{10}Ag_{90}$ discontinuous multilayer and the granular alloy samples agreed well in accordance with the observed blocking temperatures.

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Grants and international cooperations

OTKA K68612 Magnetic anisotropy of structures with reduced dimension (L.F. Kiss, 2007-2010)

Publications

Articles

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See also: E.3., H.1.

E. X-RAY DIFFRACTION

G. Faigel, F. Borondics, G. Bortel, B. Botka[#], L. Gránásy, Z. Jurek, K. Kamarás, G. Klupp, É. Kováts, L. Környei[#], K. Németh[#], G. Oszlányi, Á. Pekker[#], S. Pekker, T. Pusztai, Z. Szekrényes[#], Gy. Tegze[#], M. Tegze, H.M. Tóháti[#], Gy. Tóth[#]

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

The fullerenes are closed shell all carbon atom molecules. The most abundant among them is the C_{60} molecule. Fullerenes can form a large variety of compounds with elements or with other molecules. In the group of A_xC_{60} compounds (A=Na, K, Rb, Cs) there are materials with very interesting properties. Many superconducting materials (A_3C_{60}), and also polymers with different dimensionality (RbC_{60}, Na_4C_{60}) were found. Beside the fullerene-metal compounds there are molecular crystals formed by fullerenes and various other molecules. A family among them is the Cubane-fullerene type molecular crystals. Similarly to fullerenes Cubane (C_8H_8) is also a cage-molecule. The two type of molecules form crystals as a result of molecular recognition between the convex surface of fullerenes and the concave cubane. Static cubane occupies the octahedral voids of the face centered cubic structures and acts as a bearing between the rotating fullerene molecules. We have shown previously that the nearly ball-shaped fullerenes form cocrystals with the cube-shaped cubane and some of its substituted derivatives. The new family of molecular materials has two points of interest: a) the alternating arrays of rotating fullerene and static cubane units give rise to unusual dynamics at ambient temperatures that we called rotor-stator properties, and b) the decomposition of the highly strained cubane induces a topochemical copolymerization of the cocrystals at elevated temperatures. This year we have prepared new members of the rotor-stator family of fullerene-cubane cocrystals by building up various 1,4-disubstituted cubanes into the structures. The determination of the structures of the new materials is in progress.

We extended our earlier studies on the alkali-C_{60} compounds. We studied the catalytic activity of AC_{60} polymers on the mechanochemical dimerization of C_{60}.

Like fullerene molecules, carbon nanotubes are also exclusively built from carbon atoms. These nanostructures have many properties, which promise applications in optical, electronic and even biological systems. In order to exploit these properties, one has to characterize these materials. We continued the study of supramolecular structures by vibrational spectroscopy, specifically, the identification of hydrogen bonds by the temperature and concentration dependence of infrared spectra, and the characterization of surface-bonded conducting polymers on carbon nanotubes by infrared and Raman spectroscopy. We also studied the optical properties of carbon nanotubes under pressure.

The third type of all carbon material, which we study, is the graphene. The interest in this material is driven by its unique two dimensional character, which similarly to the carbon nanotubes promises applications in a wide area. We studied the optical properties of oriented graphene prepared by novel methods.

Theory of phase transformations. — The hard-sphere system is the best known fluid that crystallizes: the solid-liquid interfacial free energy, the equations of state, and the height of the nucleation barrier are known accurately, offering a unique possibility for a quantitative

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validation of nucleation theories. A recent significant downward revision of the interfacial free energy from ~0.61 kT/σ^2 to (0.56 ± 0.02) kT/σ^2 necessitates a re-evaluation of theoretical approaches to crystal nucleation. This has been carried out for the droplet model of the classical nucleation theory (CNT), the self-consistent classical theory (SCCT), a phenomenological diffuse interface theory (DIT), and single- and two-field variants of the phase-field theory that rely on either the usual double-well and interpolation functions (PFT/S1 and PFT/S2, respectively) or on a Ginzburg-Landau expanded free energy that reflects the crystal symmetries (PFT/GL1 and PFT/GL2). We find that the PFT/GL1, PFT/GL2, and DIT models predict fairly accurately the height of the nucleation barrier known from Monte Carlo simulations in the volume fraction range of $0.52 < \phi < 0.54$, whereas the other models underestimate it significantly.

We have extended the phase field model of heterogeneous crystal nucleation developed recently to binary alloys. Three approaches are considered to incorporate foreign walls of tunable wetting properties into phase field simulations: a continuum realization of the classical spherical cap model (called model A herein), a nonclassical approach (model B) that leads to ordering of the liquid at the wall and to the appearance of a surface spinodal, and a nonclassical model (model C) that allows for the appearance of local states at the wall that are accessible in the bulk phases only via thermal fluctuations. We illustrate the potential of the presented phase field methods for describing complex polycrystalline solidification morphologies including the shish-kebab structure, columnar to equiaxed transition, and front-particle interaction in binary alloys (Fig.1).

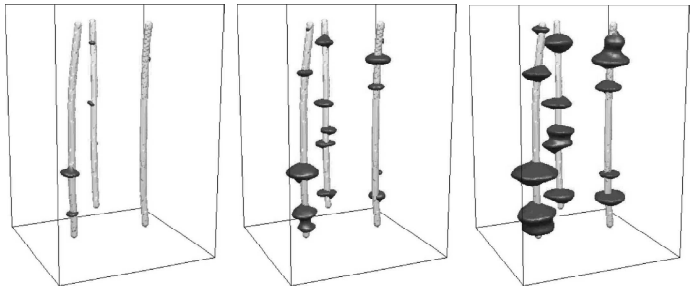

Fig. 1 *Bcc Formation of shish-kebab structure by noise-induced heterogeneous nucleation on tubular walls of contact angle $\psi = \pi/4$ in model A (see text) at T=1574 K and c_{Cu}=0.4192, in a hypothetical system whose thermodynamic properties are given by an ideal solution approximation of the Cu-Ni system. Snapshots taken at times t =30, 40, 50, and 60 μs show the walls and the solidification front (ϕ =0.5). The computation has been performed on a 200×200×300 grid.*

We have used a simple dynamical density functional approach on a diffusional time scale, to address freezing to the body-centered cubic, hexagonal close-packed, and face-centered cubic structures. We have observed faceted equilibrium shapes and diffusion-controlled layerwise crystal growth consistent with two-dimensional nucleation. The predicted growth anisotropies have been discussed in relation with results from experiment and atomistic simulations. We have also demonstrated that varying the lattice constant of a simple cubic substrate one can tune the epitaxially growing body-centered tetragonal structure between the bcc and fcc structures, and observe a Mullins-Sekerka–Asaro-Tiller-Grinfeld-type instability.

Single molecule imaging. — The bottleneck of the structure solution of biological systems is that not all specimen can be crystallized. Therefore single molecules should be measured. However, small samples are severly damaged by the measuring process itself. Even the most often used x-rays destroy the sample during the collection of a diffraction pattern. However, with the introduction of x-ray free electron laser (XFEL) sources a new

possibility will appear: one might be able to do a measurement before the atoms have time to move. This means taking a diffraction pattern within a few femto-seconds. Since these sources are not available presently, one has to model the measuring process. We joined this work, and developed a special molecular-dynamics modeling tool to describe the behaviour of the sample in the XFEL pulse. We have studied the effect of inhomogenities on the Coulomb explosion. We have shown that the deterioration of the structure is significantly larger around heavy atoms then around the light matrix atoms. Further, it was also shown that in a system with spatial density variations the first neighbor arrangement is drastically changes as compared to the homogeneous system. We also studied the first step of the data evaluation process the classification. Based on the rotational symmetry of the measurement we worked out a new classification schema. Using this method we demonstrated that it is possible to carry out the classification of 10^6 2D diffraction patterns modeled at realistic XFEL parameters.

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Grants and international cooperations

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 72954	Rotor-stator phases of the fullerene-cubane system and related supramolecular materials (S. Pekker, 2008-2012)
OTKA T 048298	Holographic methods in structural research (M. Tegze, 2005-2009)
OTKA K067980	New methods for solving the phase problem II., (G. Oszlányi, 2007-2011)
OTKA K062588	Dynamics of complex systems (T. Pusztai, 2006-2009)

ESA PECS 98043 Phase field modeling of solidification and front-particle interaction in peritectic systems (T. Pusztai, 2007–2008)

Participation in COMET K2 project A1.1.: Numerical Investigations on Dendritic Mushy Zones (T. Pusztai, 2009–2012)

Participation in EU FP6 –500635-8 project Intermetallic Materials Processing in Relation to Earth and Space Solidification (IMPRESS) (T. Pusztai, 2004–2009)

Participation in EU FP7 NMP4-SL-2008-213669 ENSEMBLE Engineered Self-organised Multi-Component Structures with Novel Controllable Electromagnetic Functionalities (L. Gránásy, 2008–2012)

NFÜ TECH-09-A2-2009-0134, FIBERSC2 Development of fiber integrated nonlinear microendoscope based on new fiber laser technology, for pharmacological and diagnostic investigations (2009-2012, consortium leader: R. Szipőcs, Scientist-in-charge for RISSPO: K. Kamarás)

EU FP6-STREP NMP4-CT-2006-031847: Towards new generation of neuro-implantable devices: engineering neuron/carbon nanotubes integrated functional units (NEURONANO) (coordinator: Laura Ballerini, University of Trieste, Italy, representative of Contractor: K. Kamarás, 2006-2009)

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)

Alexander-von-Humboldt Foundation Joint Research Project 3-Fokoop-DEU/1009755: Electronic properties of doped C_{60} and nanotube compounds, principal investigators: K. Kamarás (Hungary), Rudolf Hackl (Walther-Meissner Institute, Bavarian Academy of Sciences, Garching, Germany, 2006-2009)

Hungarian Academy of Sciences - Spanish Council for Advanced Research Bilateral ESP-18/2006 Hungarian - Spanish Intergovernmental S&T Cooperation, Investigation of pristine and intercalated carbon nanostructures (S. Pekker, 2007-2009)

Hungarian Academy of Sciences – Deutsche Forschungsgemeinschaft Joint Research Project DFG/183: Characterization of pressure-induced phenomena in carbon nanostructures (Principal investigators: K. Kamarás, Hungary and Christine Kuntscher, University of Augsburg, Germany, 2007-2009)

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See also: C.24., G.5.

F. COMPLEX FLUIDS

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

Synthesis. — We have synthesized new bent-core (BC) compounds as a continuation of our former studies. This time the double bond containing group was connected by an ester function to the core on both ends of the molecule. This ester function represents an additional polar group with the expectation to induce ferroelectric or antiferroelectric behaviour. As part of collaboration with Italian scientists we have prepared deuterium labeled bent core mesogens for 2H NMR investigations, where the isotope labeling was introduced to the central aromatic ring. In order to achieve this, a new procedure has been developed for the labeling of 4-chloro resorcinol and for the preparation of additional intermediates.

Electric field driven pattern formation. — We have reexamined the influence of the flexoelectricity on the electroconvection (EC), the effect which has previously been studied in the conductive EC regime only. Our studies have been extended to the dielectric EC regime. We have shown that flexoelectricity considerably decreases the threshold voltage of dielectric EC.

EC patterns have been studied in a thin nematic layer of very low conductivity. In this case, the dielectric EC mode persists down to very low frequencies of the driving voltage. A Lifshitz point, i.e. a transition from normal to oblique rolls, has been detected in the dielectric regime. A crossover from EC to flexoelectric domains has occurred for extremely low frequencies of about 0.1 Hz. In the crossover scenario the two pattern morphologies appear consecutively within one period of the driving voltage. A theoretical description of the onset characteristics of dielectric convection based on an extended model including flexoelectricity has also been worked out.

The onset of EC in binary mixtures of a bent-core (BC) and a rod-like nematic has been characterized by measuring the threshold voltage U_c and the critical wave number of the pattern in a wide range of frequencies f. In the mixtures rich in BC molecules a "conductive-prewavy2-patternless-prewavy1" morphological sequence has been detected with an unusual negative slope of $U_c(f)$ at high frequencies. This latter scenario seems to be related to the BC component, as it disappears with increasing the concentration of rod-like molecules. In addition, one of the parameters most relevant for electroconvection, the electrical conductivity, has also been varied by ionic salt doping. It has been found that the above effect of the BC molecules on the electroconvection scenarios can be suppressed by the conductivity.

Liquid crystal composite materials. — The 4-(trans-4'-n-hexylcyclohexyl)-isothiocyanatobenzene (6CHBT) nematic liquid crystal has been doped with multi-walled carbon nanotubes (MWNTs) and magnetically labeled MWNTs. The samples have been characterized by infrared (IR) spectroscopy, transmission electron microscopy (TEM), optical microscopy and by magnetic measurements. The electric and magnetic Freedericksz transitions have been measured for the pure 6CHBT as well as for 6CHBT doped with MWNTs or with magnetically labeled MWNTs.

Interactions at liquid crystal surfaces. — Experiments on surface reorientation of nematic liquid crystals on polyethyl-methacrylate films have shown that the time-scale of

[#] Ph.D. student

director gliding expands from a fraction of a second to several hours. A power-law distribution function of relaxation times provided very good agreement between measurements and calculated gliding curves. From the model an upper limit of the extrapolation length could be extracted, which indicated a surprisingly strong azimuthal anchoring of the liquid crystal on the polymer layer.

Light-induced optical anisotropy has been detected in azo-dye doped thin polyethyl-methacrylate films. The measured birefringence and dichroism signals have increased in an initial period of illumination, afterwards started to decrease and approached zero. Light-induced diffusion or degradation of the dye-molecules has been proposed to explain this non-monotonic behaviour of the time-dependence of the induced optical anisotropy.

Instabilities during solidification. — Crystallization of impure biphenyl has been studied in thin-sample directional solidification (T-DS) experiments. The platelike growth shape of the monoclinic biphenyl crystals includes two low-mobility (001) facets and four high-mobility {110} facets.

Upon T-DS, biphenyl plates oriented with (001) facets parallel to the sample plane can exhibit either a strong growth-induced plastic deformation (GID, see Fig. 1.), or deformation-free weakly faceted (WF) growth patterns. We determine the respective conditions of appearance of these phenomena. GID is shown to be a long-range thermal-stress effect, which disappears when the growth front has a cellular structure.

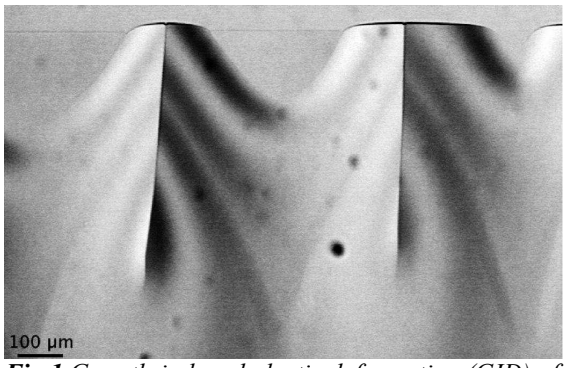

Fig.1 *Growth-induced plastic deformation (GID) of a biphenyl crystal.*

An early triggering of the cellular instability allowed us to avoid GID and study the dynamics of WF patterns as a function of the orientation of the crystal.

Granular dynamics. — Dense granular flows often become unstable and form inhomogeneous structures in nature or industry. Although recently significant advances have been made in understanding simple flows, instabilities are often not understood in detail. We have obtained experimental and numerical results that show the spontaneous formation of longitudinal stripes which arise from instability of the uniform flowing state of granular media on a rough inclined plane. The form of the stripes depends critically on the mean density of the flow with a robust form of stripes at high density that consists of fast sliding plug-like regions (stripes) on top of highly agitated *boiling* material - a configuration reminiscent of the Leidenfrost effect when a droplet of liquid lifted by its vapor is hovering above a hot surface. For further information, and movies visit the following web-site: http://www.szfki.hu/~btamas/gran/stripes.html.

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Grants and international cooperations

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

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

73ÖU2 (Austrian-Hungarian Action Foundation) New luminescent liquid crystalline monomers and oligomeres (N. Éber, 2008-2009)

NKTH TÉT 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)

MTA-ASCR (Hungarian-Czech bilateral) Synthesis and study of ferroelectric liquid crystals leading to preparation of mixtures with defined properties (K. Fodor-Csorba, 2007-2009)

MTA-CNR (Hungarian-Italian bilateral) New banana–shaped monomers and their polymer derivatives (K. Fodor-Csorba, 2007-2009)

MTA-CONACYT (Hungarian-Mexican bilateral) Investigation of dye-doped liquid crystals for photonic application (I. Jánossy, 2007-2009)

MTA-INSA (Hungarian-Indian bilateral) Experimental and theoretical studies on liquid crystals (N. Éber, 2007-2009)

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

MTA-JSPS (Hungarian-Japanese bilateral) Science and application of bent core liquid crystals (K. Fodor-Csorba, 2007-2009)

MTA-SASA (Hungarian-Serbian bilateral) Structure and physical study of bent core liquid crystals (N. Éber, 2007-2009)

MTA-SAS (Hungarian-Slovak bilateral) Stuctural phase transition in liquid crystals doped by magnetic nanoparticles (N. Éber, 2007-2009)

Long term visitors

— Shankar Rao: Centre for Liquid Crystal Research, Jallahalli, Bangalore, India, July 14-September 12, 2009 (MTA-INSA, host: Börzsönyi T)

— Prof. Antal Jákli: Liquid Crystal Institute, Kent State University, Kent, USA, June 19-July22, 2009 (host: Éber N)

— Tanya Osztapenko: Kent State University, Kent, USA, June 10-July 20, 2009 (host: Éber N.)

— Prof. David Statman: Allegheny College, Meadville, USA, June 12-July 31, 2009 (host: Jánossy I)

— Andrea N. Sharbonnel: Allegheny College, Meadville, USA, June 12-July 31, 2009 (host: Jánossy I)

— Mark W. Bordo: Allegheny College, Meadville, USA, June 12-July 31, 2009 (host: Jánossy I)

— Brandi L. Kautz: Allegheny College, Meadville, USA, June 12-July 31, 2009 (host: Jánossy I)

— Daniel R. Brennan: Allegheny College, Meadville, USA, June 12-July 31, 2009 (host: Jánossy I)

— Luis E. Aguirre: Cordoba University, Argentina, September 16-December 16, 2009 (host: Buka Á)

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Articles

F.1. Obadović* DZ, Vajda A, Jákli* A, Kohout* M, Stojanović* M, Éber N, Fodor-Csorba K, Galli* G; Phase sequences of mixtures formed by bell-shaped and calamitic compounds; *Journal of Research in Physics;* **32**, 69-74, 2008

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F.7. Fontana* J, Bailey* C, Weissflog* W, Jánossy I, Jákli* A; Optical waveguiding in bent-core liquid-crystal filaments; *Phys Rev E*; **80**, 032701, 2009

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F.10. Tóth-Katona T, Fodor-Csorba K, Buka Á; Nem légnemű, nem folyadék, nem szilárd I. (Neither gas, nor liquid, nor solid I, in Hungarian); *Természet Világa*; **140**, 358-361, 2009

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G. RADIOFREQUENCY SPECTROSCOPY

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

Graphene. — Graphene, a single of the honeycomb carbon planes of the graphite structure, is the ultimate two-dimensional electronic system in the sense of occupation of the third dimension. That in itself would justify interest, but its major drawing point is a solid state manifestation of relativistic-like dynamics which sets it apart from the classic Newtonian dynamics two-dimensional systems which have interested us to date in the form of semiconductor heterojunctions or electrons on the surface of liquid helium.

Experimentally, graphene was discovered, or should one say uncovered, in 2005 and very quickly shown to have electronic properties characteristic of massless fermions by the sequence of Shubnikov magnetoresistance oscillations and quantum Hall effect plateaux. It also has the unique feature of being continuously tunable by capacitive charge transfer from electron excess to electron deficient (hole) states while maintaining a non-zero minimum conductivity at the neutrality point.

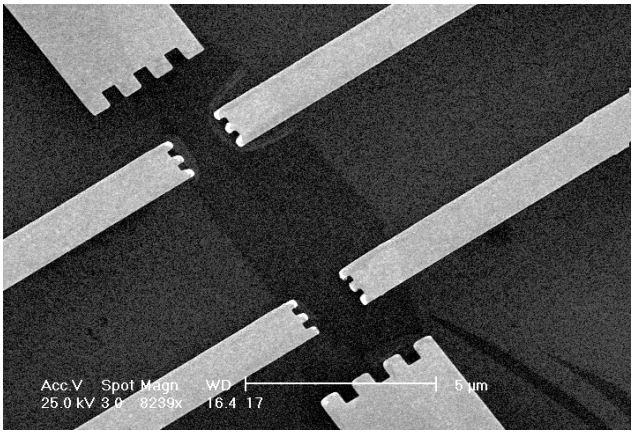

Fig. 1 *Scanning electron microscope image of contacted graphene sample. The sample is the dark patch of about 7 x 3 μm^2.*

Our activity to date in the domain of graphene, apart from organizing a local discussion forum, has been to learn how to fabricate samples from our Saclay colleagues and to investigate their magnetoresistive properties in our Budapest laboratory. We see this as a prelude to more original experiments on edge magneto-plasmon propagation at 40-60 GHz, again in collaboration with the Service de Physique de l'Etat Condensé (SPEC) Saclay.

Hydration of intrinsically disordered proteins. — Wide-line ^{1}H NMR has been extensively used for the study of protein systems in order to better understand the structure and dynamics of the protein-water (protein-solvent) interfacial region and its relationship with the protein structure and function. The analysis of the nuclear relaxation rates supplies information on the active relaxation channels and gives the relevant coupling constants, activation energies, and correlation times.

The human ubiquitin and bovine serum albumin were used as references for globular proteins and the intrinsically disordered α- and β-caseins, and the amyloid fiber forming proteins α-synuclein and β_2-microglobulin were investigated. The rates of spin-lattice, spin-spin and rotating-frame spin-lattice relaxation were measured in the temperature range -70 to +40°C. Protein solutions were prepared with pure water and buffered (150 mM NaCl, 50 mM TRIS and 1 mM EDTA) solutions.

The interfacial water can be examined this way from a variety of aspects. The magnitude of the coupling constant can be used as a guide to decide about the interactions governing the relaxation, and it provides information on the geometry. The activation energy tells

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about the thermodynamic relations of the molecular reorientations while the correlation time is about the dynamics.

The general feature was found for all proteins studied to date that the activation energy for the interfacial water is substantially lower for the pure water solutions than for the buffered solutions. The corresponding correlation times are shorter by orders of magnitude for the buffered solutions than for the pure water solutions. These differences reveal the cosolutes are not independently hydrated. Consequently, the generally used relaxation model by which the dipole-dipole interaction is considered only is insufficient. The effects of the solvent accessible protein surface and the other solutes as ions on the ^{1}H spin system of the interfacial water should be considered as well in the frame of a more complete and detailed model. The comparison between the relaxation behavior of the globular and intrinsically disordered proteins showed that the disordered proteins are in more intensive interactions with the salt ions than the compact globular proteins. It follows that the intrinsically disordered proteins have larger ion-sink capacities, a most important aspect in their biological functions.

Differential Scanning Calorimeter for microliter samples. — Differential Scanning Calorimetry (DSC) is a method that allows for precise determination of the enthalpy of transition and changes in heat capacity from the recorded temperature differences, ΔT, between the reference and sample branches. We have developed a DSC model for the investigation of biological systems that are in a form of low concentration aqueous solutions of proteins. The temperature range achieved is from deeply frozen (-170°C) up to above the boiling point of water. This temperature range allows for separating different types of water: free bulk, protein surface bound, and glassy.

Fig. 2a *Top view of the calorimeter with the silver heat-leak disk*

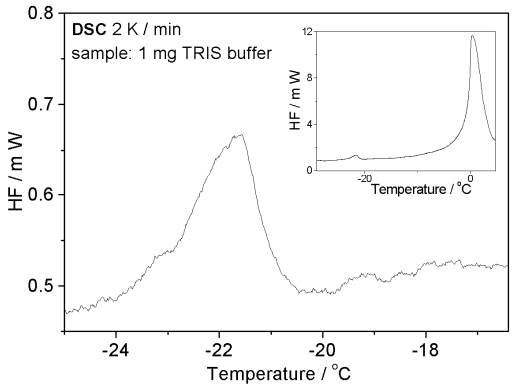

Fig. 2b *Thermograph of the melting of the eutectic of 1 µliter TRIS buffer*

The instrument is based on the classical design of heat-flux differential calorimeters. The left panel of Fig. 2 displays a top view of the heat-leak disk made of silver. The reference and sample crucibles are placed on it and are separated by constantan bridges that permit a lag in temperature proportional to the heat capacity. In Fig. 2b, a thermograph of the melting of the eutectic of 1 µliter TRIS buffer is depicted.

The flexibility of programming makes the calorimeter applicable in many other fields such as low-temperature metal physics, polymer science, purity analysis, and quality testing. The instrument is very suitable for students and young researchers interested in the study of experimental thermal analysis and in the creation new experiments applying specialized

temperature profiles (temperature modulation or stepwise temperature increase), external magnetic fields, etc.

Installation of a new NMR console. — We have purchased and installed a Bruker Avance III NMR console to use in our 9-T spectrometer. In cooperation with the manufacturer, we have integrated seamlessly this state-of-the-art equipment with our existing magnet system, cryogenic probes and amplifiers. The new system provides us with more flexibility in designing experiments, improved signal-to-noise ratio, faster operation and the possibility of introducing new spectroscopic techniques.

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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)
OTKA K 62280	Phase transitions in correlated electron systems: Theory and NMR experiments (project leader: K. Penc; participant: M. Bokor; 2006-2009)

Publications

Articles

G.1 Balázs* A, Csizmok* V, Buday* L, Rakács* M, Kiss* R, Bokor M, Udupa* R, Tompa K, Tompa* P; High levels of structural disorder in scaffold proteins as exemplified by a novel neuronal protein, CASK-interactive protein1; *FEBS Journal* **276**, 4168-4180, 2009

G.2 Kriza G, Pallinger Á, Sas B, Pethes* I, Vad* K, Williams FIB; Bardeen–Stephen flux flow law disobeyed in $Bi_2Sr_2CaCu_2O_{8+\delta}$; *Physica B;* **404**, 510-512, 2009

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Other

G.7. Kamasa P, Bokor M, Tompa K; Identification the type of mobile water in frozen NaCl, KCl aqueous and tris buffered solutions by DSC and NMR methods; in: *Proc. Sci. Conf. Physics of Materials*; Eds. V. Lisý and D. Olčák, Faculty of Electrical Engineering and Informatics, TU Košice, Slovakia, pp. 104-108, 2009

H. ELECTRODEPOSITED NANOSTRUCTURES

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

Depth profile analysis of electrodeposited alloys. — 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 Fe-Co-Ni alloys starts with an iron-rich zone. The iron concentration in the deposit decreases with the sample thickness, while a concominant increase in Co and Ni concentrations can be seen. This initial zone ranges to about 150 nm, which is followed by the bulk deposit where systematic concentration changes no longer occur. This spontaneous zone formation was confirmed for all electrolyte compositions used for the Fe-Co-Ni alloy deposition.

The formation of the initial Fe-rich zone can be explained by the depositon preference of the iron-group metals. The deposition starts with the most preferred metal (Fe), and the vicinity of the cathode starts to be depleted for the Fe^{2+} ions. Hence, the current could be maintained with the increase in the deposition rate of the rest of the alloy components. Therefore, the spontaneous zone formation in the near-substrate zone is the consequence of the deposition preference and the impact of diffusion of the reactant in the electrolyte on the deposition rate of each metal.

Structure and giant magnetoresistance (GMR) of electrodeposited multilayers. — The formation of microstructural defects during the growth of electrodeposited Co/Cu multilayers was investigated using the combination of wide-angle and small-angle X-ray scattering and HRTEM in collaboration with the Technical University Freiberg, Germany. Generally, the microstructural analysis confirmed the development of periodic multilayer structures which were mainly of fcc type but contained some hcp fraction of cobalt and large, highly cumulative interface corrugations. A detailed analysis of the microstructural defects in the ED Co/Cu multilayers with a nearly constant thickness of Co layers has shown that the defect type depends strongly on the thickness of the copper layers. Extremely thin and, hence, discontinuous Cu layers were found to be compressed, which was due the lattice misfit between cobalt and copper. Moreover, in the ED Co/Cu multilayers with extremely thin Cu layers, the Co layers contained (001)- and (100)-oriented hcp cobalt and (100)-oriented fcc cobalt. The existence of crystallites with these orientations and the atomic arrangement at the boundaries between crystallites of different orientations were the main sources of the microstructural defects in such multilayers. The increasing thickness of the Cu layers stabilized the fcc structure in the Co layers and reduced the elastic deformation in copper, which was originally induced by the lattice misfit between cobalt and copper. This relaxation of the residual stresses happened through the formation of microtwins that were oriented perpendicularly to the growth direction.

In order to clarify the controversial results reported in the literature for the spacer layer thickness dependence of GMR in electrodeposited multilayers, a detailed study of the GMR evolution was performed on Co/Cu multilayers prepared under controlled electrochemical conditions with Cu layer thicknesses ranging from 0.5 nm to 4.5 nm. It turned out that for thin Cu layers (up to 1.5 nm) AMR occurs. This could be explained by a high density of pin-holes in the thin spacer layers (as evidenced by the above described

[#] Ph.D. student

structural studies) that enable the percolation of the magnetic layers yielding an overall bulk ferromagnetic (FM) like behaviour manifested in the observed anisotropic magnetoresistance (AMR) as shown in Fig. 1. For thicker Cu layers, a clear GMR was observed the magnitude of which increased up to a maximum at about 3.5 to 4 nm and with a slight decrease afterwards. The results of coercive field and zero-field resistivity measurements (Fig. 2) also indicated a transition from Cu layers with a high density of pin-holes to Cu layers with much better continuity and/or thickness uniformity at comparable thicknesses as deduced from the magnetoresistance data. According to magnetic measurements up to 50 kOe, the relative remanence for an AMR and a GMR multilayer was practically the same, hinting at the absence of an AF coupling between the magnetic layers. With increasing continuity and thickness uniformity of the thicker and thicker spacer layers, the FM coupling strength is gradually reduced and finally disappears. This results in completely uncoupled magnetic layers with random magnetization orientations. As the magnetic layers become more and more randomly aligned with diminishing FM coupling, electron transitions between them provide an increasing GMR effect for larger spacer layer thicknesses.

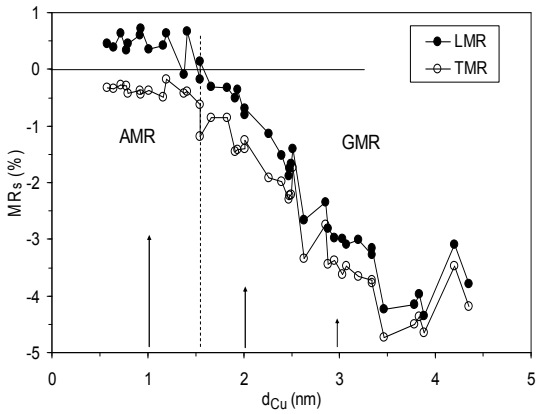

Fig. 1 *Evolution of the longitudinal (LMR) and transverse (TMR) saturation components of the magnetoresistance MR for the investigated electrodeposited Co/Cu multilayers as a function of the Cu layer thickness d_{Cu}. The vertical dashed line separates the AMR and GMR thickness ranges. The vertical arrows denote the approximate positions of the GMR maxima reported for fcc(111) Co/Cu multilayers prepared by physical deposition methods.*

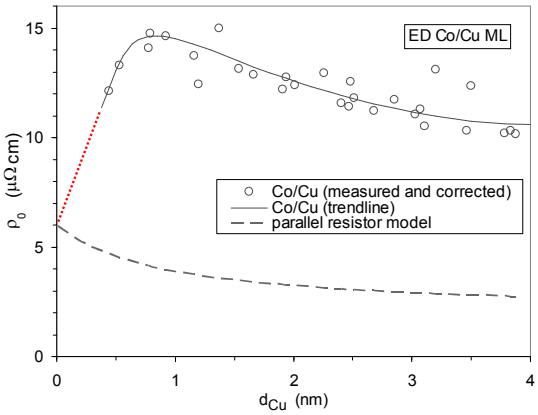

Fig. 2 *Room-temperature electrical resistivity (ρ_0) of electrodeposited Co/Cu multilayers in zero external magnetic field as a function of the Cu layer thickness with constant magnetic layer thickness $d_{Co} \approx 2.7$ nm. The dashed line represents the resistivity of a Co/Cu multilayer in a simple parallel resistor model, calculated with bulk resistivity values of the individual layers. The dotted line is just a linear extrapolation of the experimental data to $d_{Cu} = 0$.*

As a main conclusion, it is believed that the absence of oscillatory GMR in electrodeposited multilayers is (i) partly due to the microstructural features revealed which features result in an FM coupling for a very large range of spacer layer thicknesses and (ii) partly due to the absence of a significant AF coupling between the adjacent layers at the appropriate layer thicknesses.

Submicron-scale processes in geomaterials. — Remnants of numerous processes which have not reached thermodynamic equilibrium are preserved in rocks. They provide useful information on the evolution of the lithosphere and interactions between different geospheres. Mineral reactions observed in nature play an important role in the understanding of slow chemical reactions in solid-phase materials since their duration is orders of magnitude longer than laboratory experiments. Our research interest is focused on the mechanisms and kinetics of microstructure evolution and the development of submicron-sized chemical heterogeneities during chemical reactions between solid phases.

Numerical models are developed to simulate element distribution and microstructure evolution recorded in minerals from natural samples. All these investigations are carried out in collaboration with the Free University of Berlin, Germany and the Eötvös Loránd Geophysical Institute of Hungary, Budapest.

Submicron-sized chemical zoning patterns have been detected in Fe-Ti-oxides formed in the lower crust by means of high-resolution electron-beam microanalytical techniques. We have found that the composition of these minerals was modified due to the interaction with the magma which transported these rocks to the surface. By the numerical modelling of diffusion-controlled Fe–Ti exchange within these oxides, we estimated the maximum magma ascent rate to be 9-20 hours / 30 km. In addition, we gave a first estimation of the Fe-Ti interdiffusion coefficient of ilmenite based on these samples.

The breakdown of a silicate mineral (garnet) was also studied using high-resolution electron-beam microanalytical techniques. The reaction includes the replacement of a homogeneous precursor phase along a moving interphase boundary by three different nanometer-sized phases forming vermicular intergrowths (symplectitic microstructure). Oriented transmission electron microscopy (TEM) foils were prepared from the reaction products parallel with and perpendicular to the reaction interface by focused ion beam technique. A TEM study of these samples provided new information on the mechanism of phase separation along a moving reaction front in the solid phase. 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 K 61182 Fluids in the lithosphere of the Bakony-Balaton Highland Volcanic Field (Principal investigator: K. Török, Eötvös Loránd Geophysical Institute of Hungary; SZFKI participant: J. Dégi; 2006 –2009)

International collaboration with the FOR 741 DFG research unit: Nanoscale processes and geomaterial's properties (Project leader: R. Abart, Free University, Berlin, Germany, SZFKI participant: J. Dégi; 2007 –2009)

Publications

Articles

H.1. Bakonyi I, Simon E, Tóth BG, Péter L, Kiss LF; Giant magnetoresistance in electrodeposited Co-Cu/Cu multilayers: origin of the absence of oscillatory behavior; *Phys Rev B;* **79**, 174421/1-13, 2009

H.2. Bartók A, Csik* A, Vad* K, Molnár* G, Tóth-Kádár E, Péter L; Application of surface roughness data for the evaluation of depth profile measurements of nanoscale multilayers; *J Eletrochem Soc.;* **156**, D253-D260, 2009

H.3. Csik* A, Vad* K, Tóth-Kádár E, Péter L; Spontaneous near-substrate composition modulation in electrodeposited Fe-Co-Ni alloys; *Electrochem Commun;* **11**, 1289-1291, 2009

H.4. Dégi J, Abart* R, Török* K, Rhede* D, Petrishcheva* E.; Evidence for xenolith-host basalt interaction from chemical patterns in Fe-Ti-oxides from mafic granulite xenoliths of the Bakony-Balaton Volcanic field (W-Hungary); *Mineralogy and Petrology*; **95**, 219-234, 2009

H.5. García-Torres J, Péter L, Révész* Á, Pogány L, Bakonyi I; Preparation and giant magnetoresistance in electrodeposited Co-Ag/Ag multilayers; *Thin Solid Films;* **517**, 6081-6090, 2009

H.6. Rafaja* D, Schimpf* C, Klemm* V, Schreiber* G, Bakonyi I, Péter L; Formation of microstructural defects in electrodeposited Co/Cu multilayers; *Acta Mater.;* **57**, 3211-3222, 2009

H.8. Bakonyi I, Péter L; Electrodeposited multilayer films with giant magnetoresistance (GMR): progress and problems; *Progr. Mater. Sci.*; accepted for publication, DOI: 10.1016/j.vacuum.2009.04.066

H.9. Csik* A, Vad* K, Langer* GA, Katona* GL, Tóth-Kádár E, Péter L; Analysis of Co/Cu multilayers by SNMS reverse depth profiling; *Vacuum;* accepted for publication, DOI: 10.1016/j.pmatsci.2009.07.001

H.10. 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.*; accepted for publication, DOI: 10.1007/s00410-009-0428-z

Book chapter

H.11. Péter L, Bakonyi I; In: *Nanomagnetism and Spintronics: Fabrication, Materials and Characterization, and Applications*; Eds.: Nasirpouri F and Nogaret A, (World Scientific, Singapore, 2010), accepted for publication; ISBN: 978-981-4273-05-3, http://www.worldscibooks.com/nanosci/7281.html

Others

H.12. Péter L; A mítosz varázsa (Fascination of the myth, in Hungarian); *Magyar Tudomány*; accepted for publication

See also: R.4.

I. METALLURGY AND MAGNETISM

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

Metallurgy. — Besides studying glass forming ability (GFA), we have tried to assess also the high-entropy alloy forming ability (HEA-FA) by constructing diagrams which represent the alloy formation enthalpy (ΔH) versus the atomic size mismatch (δ). Surveying the data available from the literature and adding new data for more than 30 alloy compositions studied by our group, it turned out that in order to obtain ductile Al-based metallic glasses (MG's) containing more than 75-80 at.% Al, one has to select alloying elements for which the heats of formation (ΔH) are between -5 and -25 kJ/mole. In addition, we have found new amorphous Al-based compositions on the basis of the assumption that the higher the number of stable and metastable phases in the surrounding of the selected composition, the higher the GFA is. Nevertheless, we have to exclude those alloying elements which form compounds with high Al-content, above 80 at.%. Concerning HEA-FA, it is generally accepted that for obtaining a crystalline solid solution, both the atomic mismatch (δ) and the free energy (ΔG) should be small enough in order to avoid that the solute element forms compound-like precipitates. The free energy can be diminished by increasing the configurational entropy (ΔS) in a manner that a multicomponent alloy is composed by using equal atomic concentrations of at least 5 constituents:

$$\Delta S = R \cdot \sum_i c_i \cdot \ln c_i$$

This idea proved to be valid for the mixing of the late transition elements (Cu, Ni, Co, Fe, Cr) and their derivatives. In the case of Al- and Ti-based multicomponent alloys, however, an extended solid solution was observed only for components which form no compound phases.

Soft magnetic nanocrystalline alloys. — The induced magnetic anisotropy by magnetic field and mechanical stress-annealing was used for tailoring the properties of nanocrystalline soft magnetic cores for electrical noise suppression applications. Transformer cores of different outer and inner diameters ranging from 20 to 220 mm have been tested for our industrial partners. Mössbauer study of stress-annealed Finemet type ribbon samples revealed the out-of-plane rotation of the magnetic moments as a function of the applied stress.

Micro-probe head for simultaneous DTA and TMAG measurements on sub-milligram samples. — Changes during magnetic phase transformations of ferromagnetic materials can be investigated by thermomagnetic analysis (TMAG). On the other hand, structural changes of materials resulting in changes of macroscopic thermal properties such as heat capacity or latent heat can be detected by differential scanning calorimetry (DSC) or differential thermal analysis (DTA). The measurement of changes in the magnetic and thermal properties is usually realized in separate experiments. At the moment, there is no commercially available instrumentation for simultaneous thermal and thermomagnetic analysis. To fill the gap, a micro probe-head was developed in our laboratory for simultaneously recording thermal and magnetic properties of the material under study for small samples with masses below 1 mg. The instrumentation allows to

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detect the changes in the magnetic and thermal properties of a given sample under investigation in the same equipment and experiment. The main advantage of the method realized by the apparatus is the ubiquitous determination of the sample temperature during transition, while the significant uncertainty is associated with results from separate TMAG and DSC/DTA experiment. In this way the magnetic and thermal changes are recorded against the same sample temperature, avoiding the uncertainty connected with measurements carried out in separate equipments.

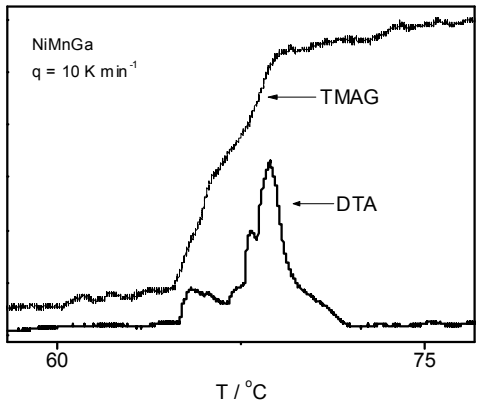

Fig. 1 *Results obtained for a Ni-Mn-Ga type shape-memory alloy*

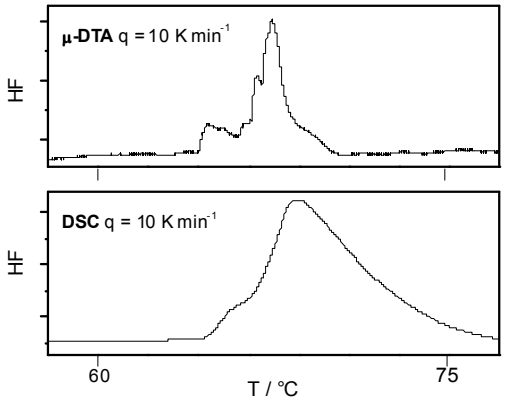

Fig. 2 *Micro-DTA and conventional DSC of a Ni-Mn-Ga type shape-memory alloy*

As an example, the results obtained for a Ni-Mn-Ga type shape-memory alloy are presented in Fig. 1. The steep uprise of magnetization at 67.4 ˚C (TMAG curve) corresponds to a martensite-austenite (M-A) structural transformation which manifests itself in a pronounced exothermal latent heat in the DTA curve. The DTA recorded by the micro-probe head reveals a multistage transformation the details of which are not resolved by the conventional DSC performed on the same sample (Fig. 2).

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Grants and international cooperations

OTKA K62466 Investigation of the deterioration of power plant construction materials by magnetic methods (Project leader: J. Ginsztler (BME), SZFKI participant: L.K. Varga, 2006-2009)

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. Development of magnetic field annealing for the inductive electronic component market (Project leader: L.K. Varga, 2009)

Publications

Articles

I.1. Kane* SN, Gercsi* Zs, Mazaleyrat* F, Varga LK, Coisson* M, Tiberto* P, Vinai* F, Celegato* F, Jeong* YH; Influence of composition and thermal treatments on structural, magnetic and magnetotransport properties of $(Fe_{100-x}Co_x)_{78}Si_9Nb_3B_9Cu_1$ alloys; *J Korean Phys Soc;* **53**, 3634-3639, 2008

I.2. Kane* SN, Khinchi* SS, Gercsi* Zs, Gupta* A, Varga LK, Mazaleyrat* F, Jeong* YH; Structural and magnetic investigation of amorphous and gradually devitrified nanocrystalline Fe-Co-Nb-Cu-B alloys, *J Korean Phys Soc;* **53**, 3629-3633, 2008

I.3. Fazakas É, Kane* SN, Lázár* K, Varga LK; Mössbauer study of rapidly solidified Al-Fe based amorphous alloys; *Hyperf Int;* **189**, 119-123, 2009

I.4. Fazakas É, Russew* K, Stojanova* L, Csanády* Á, Varga LK; $Al_{85}Ta_6Ni_9$, a refractory Al-rich ternary alloy glass and its crystallization kinetics; *J Phys: Conf Series;* **144**, 012100/1-4, 2009

I.5. Fazakas É, Varga* B, Varga LK; Study of amorphous-crystalline phase transformations by dilatometer in the case of $Al_{88}Y_7Fe_5$ and $Al_{88}Y_7Fe_4Sb_1$ amorphous alloys; *Metalurgia (Romania)*; **61**, 5-7, 2009

I.6. Henits* P, Kovács* Zs, Varga LK, Révész* Á; Nanocrystallization in $Al_{85}Ce_8Ni_5Co_2$ amorphous alloy induced by heat treatment and severe plastic deformation; *J Phys: Conf Series;* **144**, 012095/1-4, 2009

I.7. Kane* SN, Alves* F, Gupta* A, Gupta* P, Varga LK; Study of rapid stress annealed nano-crystalline $Fe_{74.5}Cu_1Nb_3Si_{15.5}B_6$ alloy; *Hyperf Int;* **191**, 47-53, 2009

I.8. Kane* SN, Khinchi* SS, Mazaleyrat* F, Gercsi* Z, Gupta* A, Varga LK; Study of structural and magnetic properties of Co-substituted $(Fe_{100-x}Co_x)_{78}Si_9Nb_3B_9Cu_1$ alloys; *J. Phys: Conf Series;* **144**, 012078/1-4, 2009

I.9. Kane* SN, Lee* HJ, Jeong* YH, Varga LK; Cast iron (CI) based soft magnetic BMG $Ci_{88.3}Al_2Ga_1P_{4.35}B_{4.35}$; *J Phys: Conf Series;* **144**, 012040/1-4, 2009

I.10. Kane* SN, Lee* HJ, Kim* SB, Jeong* YH, Hyun* SW, Kim* CS, Varga LK; Effects of B and P content on structural and magnetic properties of cast iron based amorphous alloys; *Hyperf Int;* **191**, 109-113, 2009

I.11. Kolano-Burian* A, Kolano* R, Varga LK; Magnetically induced anisotropy in Co rich Finemet type nanocrystalline alloys; *J All Comp;* **483**, 560-562, 2009

I.12. Russew* K, Stojanova* L, Varga LK, Fazakas É, Yankova* S; Glass forming ability and thermal behavior of binary Co-Zr amorphous alloys; *J Mater Sci Technol;* **17**, 29-36, 2009

I.13. Russew* K, Stojanova* L, Yankova* S, Fazakas É, Varga LK; Thermal behavior and melt fragility number of $Cu_{100-x}Zr_x$ glassy alloys in terms of crystallization and viscous flow; *J Phys: Conf Series;* **144**, 012094/1-4, 2009

I.14. Varga* B, Fazakas É, Hargitai* H, Varga LK; Dilatometer study of rapidly solidified aluminium-silicon based alloys; *J Phys: Conf Series;* **144**, 012105/1-4, 2009

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I.15. Stojanova* L, Yankova* S, Fazakas É, Varga LK, Russew* K; Thermal stability and mechanical properties of Al-U based amorphous alloys (in Bulgarian); In: *Proc. 24th Natl. Conf. on Non-Destructive Testing (Sozopol, Bulgaria, 2009). Nauchno-tekhnicheski Soyuz po Mashinostroeniya (Bulgaria)*; **16**, 260-266, 2009

I.16. Stojanova* L, Yankova* S, Fazakas É, Varga LK, Russew* K; Thermal behaviour of $Al_{100-x}Y_x$ amorphous alloys (in Bulgarian); In: *Proc. 24th Natl. Conf. on Non-Destructive Testing (Sozopol, Bulgaria, 2009). Nauchno-tekhnicheski Soyuz po Mashinostroeniya (Bulgaria);* **16**, 267-272, 2009

Book

I.17. Csanády* Á, Kálmán* E, Konczos G. (Eds.); *Bevezetés a nanoszerkezetű anyagok világába (Introduction into the world of nanostructured materials*, in Hungarian); ELTE Eötvös Kiadó, Budapest, 2009, pp. 1-313.

Others

I.18. Fazakas É, Varga* B, Varga LK; Dilatométerrel és DSC-vel vizsgált amorf kristályos fázisátalakulások aluminium ötvözetekben (Study of structural changes of aluminium based amorphous alloys by DSC and dilatometer, in English); in: *Proc. 11th Mining, Metallurgy and Geology Conference (Sighetu Marmatiei, Romania, 2009)*; Hungarian Technical Scientific Society of Transylvania; pp. 190-194, 2009

See also: G.4., G.7.

J. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

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

Neutron holographic measurement on ammonium-chloride. — We have made a succesfull neutron holographic measurement on ammonium-chloride (NH_4Cl) on the thermal three-axes spectrometer (TAST) at the 8-th thermal neutron channel of the Budapest Research Reactor (BRR). In this measurement the protons act as internal detector and internal source of neutrons also. The simultaneously appearing inside detector and inside source hologram cause false peaks, but increase the signal-to-noise ratio. We have measured the hologram at 45° scattering angle, and rotated the sample around two axes using an Eulerian cradle. The plane of the cradle was parallel to the scattered beam. For the better signal-to-noise ratio we have put the detector close to the sample. Its total viewing angle was near 5°. The angular steps were also 5° in both direction. The reconstructed holographic peaks of the first nitrogen and first hydrogen neighbours of the hydrogen atoms are in good agreement with the model calculations.

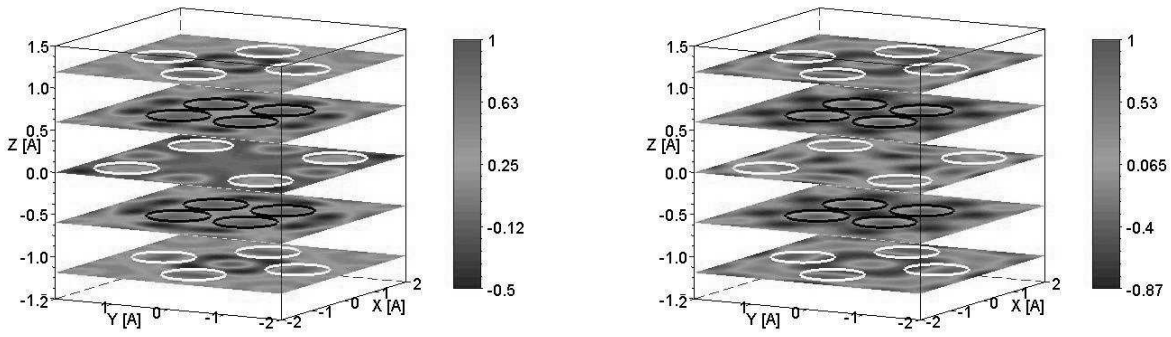


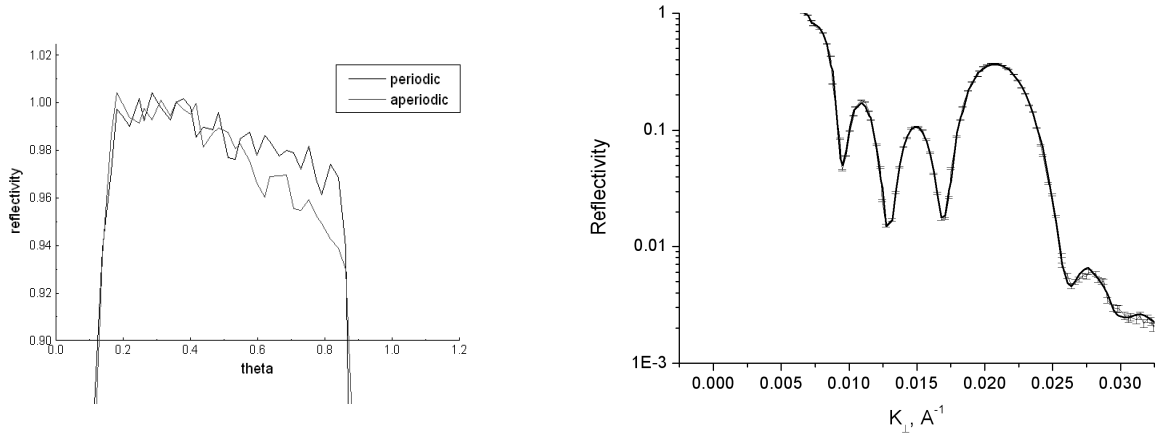
Fig. 1 *Reconstructed holographic image of ammonium-chloride from the measurement (left side) and from the model calculation (right side). The positions of hydrogen and nitrogen atoms are signed by white and black circles, respectively. In the middle layer the false peaks out of the circles are the artefacts caused by the simultaneously appearing inside detector and inside source hologram.*

Investigation of periodic multilayers. — The recipe used nowadays in the neutron supermirror production gives aperiodic multilayers. The thickness of the consecutive layers is changing from bilayer to bilayer. A new algorithm proposed by V. Ignatovich and I. Carron gives periodic supermirrors in the sense, that they are composed of periodic stacks of bilayers. The realization began in the cooperation of SZFKI, Mirrotron Ltd (Budapest) and JINR (Dubna). Already the first produced supermirrors have similar (sometimes better) reflectivity as the traditional ones under the same conditions (same sputtering machine, similar number of layers).

Fig.2 (a) shows the reflectivity of a periodic and aperiodic supermirror as function of incidence angle, λ=4.28 Å. Fig.2 (b) shows the measured (bars) and fitted (line) reflectivity of a periodic multilayer. To study the imperfectness of the produced layers simple periodic multilayers were also produced which give Bragg reflection at 2 $\theta_{crit\ Ni}$. According to this condition, the thickness of Ni layers is 84 Å, and 70 Å for the Ti layers. The number of layers is 4, 8 and 16. From these specular reflectivity curves, measured at

[#] Ph.D. student

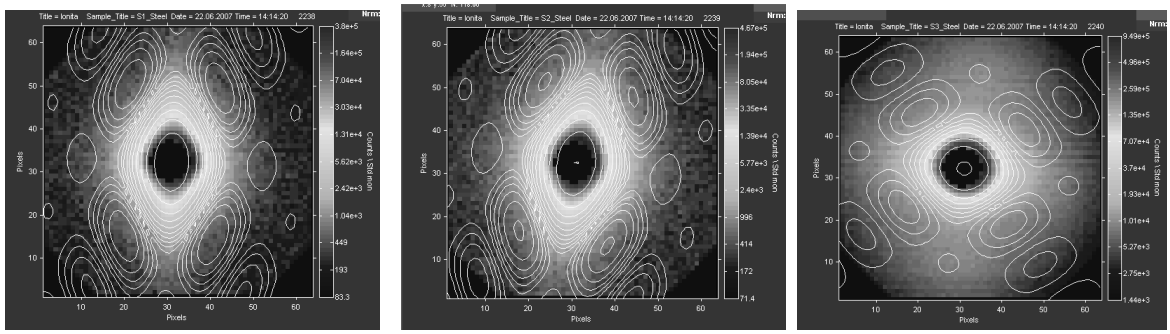
BNC, the real layer thicknesses and scattering densities were calculated. To investigate the roughness of the interfaces we also measured the off-specular scattering at GKSS, Geesthacht, Germany.



(a) (b)

Fig. 2 *(a) Reflectivity of a periodic and aperiodic supermirror as function of incidence angle, λ=4.28 Å. (b) Measured (bars) and fitted (line) reflectivity of a periodic multilayer*

Investigation of steels. — We have investigated by small angle neutron scattering (SANS) a duplex steel (containing two different phases) of industrial interest subjected to various ageing processes. Supposing that the scattering objects in steels have cuboid or rombohedral form, the scattering law obeys known formulae (in the case of monodisperse size distribution) and the characteristic size of these particles can be determined. The form factor and the contrast factor of the objects relative to the basic material give information also on the angle of orientation of the diagonal of the rhombes relatively to the main axes of investigation. We have observed the growth of cuboids with size changes from $a \approx 17$ *nm* to $a \approx 20.5 \pm 6.6$ *nm* due to thermal treatment. Further thermal treatment causes a developing of polydispersity of scattering particles. Therefore in this case only an average size was estimated. It was shown that this system becomes very polydisperse and the scattering data can be approximated by average parameter of particles as $a \approx 17$ *nm.*



(a) (b) (c)

Fig. 3 *SANS analysis of steel samples (a) S1 as received, (b) S2 aged at low temperature, (c) S3 aged at high temperature. This yields the characteristic thermal treatment to evaluate the aging process.*

Neutron instrumentation. — The 10 MW Budapest Research Rector (BRR) with its experimental facilities on the KFKI site is a unique large-scale facility in the Central European region and the basis for domestic and international user community to serves for basic and applied research as well as for instrument development. 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 application of high class detectors. In order to satisfy the need of high efficiency neutron detection of our department, significant effort was applied to develop large area position sensitive neutron detectors. The main goal of such an effort is to produce detector sensitive area of approximately half square meters which corresponds to linear size of 500x800 mm^2. The readout principle is based on the delay-line method. The applied length of the delay line was equal to 300nsec. The data collection system consisting of a preamplifier-constant fraction discriminator – time digital converter allowed to achieve the local count rate 50 kHz while the global count rate limit is 300kHz. The main parameters of this detector were determined on the cold neutron beams 10/1 and 10/3 of BRR.. It has been shown that the efficiency of the detector at wavelegth 3.14 Å is equal to 74%. The spatial resolution is 3.8 mm FWHM. The homogenity of the detector varied over the total sensitive surface between the limits ± 10%. This variation can be smoothed out by applying a normalization procedure based on a homogeneus illumination of the detector surface. Every pixel of the normalizing image contained about 10^6 counts, corresponding to a relative statistical error of 0.1%.

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Grants and international cooperations

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

EU-FP7-Charisma - Cultural heritage advanced research infrastructures: Synergy for a multidisciplinary approach to conservation/restoration (L. Rosta, 2009-2013)

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

IAEA 13507 Improvement of neutron beam performance and sample environment in residual stress (Gy. Török 2006-2009)

NAP VENEUS-2009 OMFB-06482/2009 Visegrád Cooperation for Development and Application of Neutron Spectroscopy Techniques in Multidisciplinary Research (L. Rosta, 2009-2011)

Long-term visitors

— Lilia Elnikova, Alikhanov Institute for Theoretical and Experimental Physics, Moscow, Russia, September 15, 2008 - April 30, 2009 (host: L Almásy)

— G. Pépy, Laboratoire Léon Brillouin (LLB), CEA Saclay, France, February 8-25, October 5 - November 21, 2009 (host: L. Rosta)

Publications

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J.1. Káli Gy, Sánta Zs, Bleif* HJ, Mezei F, Rosta L, Szalók* M; Commissioning of the high resolution TOF diffractometer at the Budapest Research Reactor; *Zeitschrift für Kristallographie*; Part 1 Suppl 26, 165-170, 2007

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J.27. Zamponi* M, Pyckhout-Hintzen* W, Monkenbusch* M, Wischnewski* A,Willner* L, Richter* D, Káli Gy; Branch point motion in star polymer melts; In: *Proc. International Conference on Quasielastic Neutron Scattering: Paul-Scherrer-Institut, Laue-Langevin, Schweiz, 10.02- 13.02.2009*; accepted for publication

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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

Multiferroic ortoferrites. — Samples from the mixed oxide system $YCr_{1-x}Fe_xO_3$ ($0 \le x \le 1$) were prepared by self-propagation combustion techniques and studied by neutron and X-ray diffraction at 290 K and by magnetic measurements in the range 2–800 K. The average observed metal-oxygen distances based on refinements in the space group Pnma (see Fig. 1) are in agreement with the expected distances from the valence bond approach. The non-collinear spin arrangement (mode Γ4) of $YFeO_3$ and $YCrO_3$ is preserved for the rest ($x \ge 0.33$) of the compounds magnetic at 290 K. The findings indicate that $YCrO_3$ and $YFeO_3$ form a solid solution with strongly frustrated magnetic interactions.

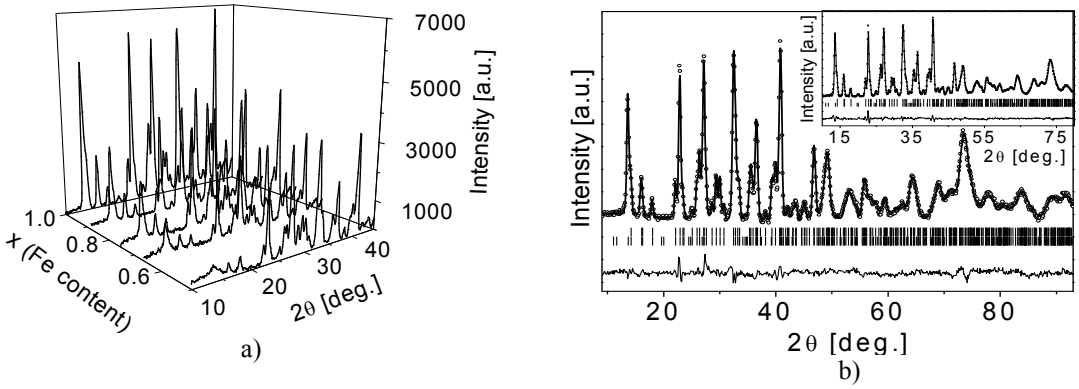

Fig. 1 *a) Low angle part of room temperature neutron diffraction patterns of $YCr_{1-x}Fe_xO_3$; b) Full profile refinement of $YFe_{0.875}Cr_{0.125}O_3$ and $YFeO_3$ (inset) (λ= 1.069 Å).*

Manganites. — Fe-substituted manganites $Bi_{0.5}Sr_{0.5}Fe_xMn_{1-x}O_3$ ($0 \le x \le 1.0$) were synthesized by a solid-state reaction. X-ray powder diffraction and neutron diffraction investigations performed at room temperature show that the crystal structure is orthorhombic for $x \le 0.3$ (see Fig. 2) and cubic for $x > 0.4$. The magnetic state of the compounds with different Fe contents changes from paramagnetic to weak antiferromagnetic below the temperature T_N varying in the range of 115–155 K. Unusual thermomagnetic behavior in the paramagnetic region was observed, which could be related to a coexistence of antiferromagnetic and ferromagnetic fluctuations far above T_N.

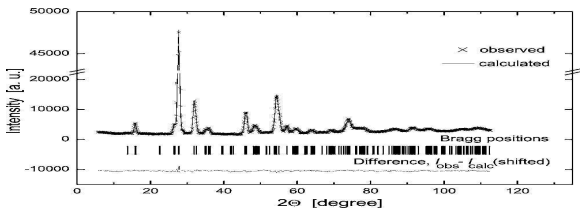

Fig. 2 *Neutron diffraction pattern of $Bi_{0.5}Sr_{0.5}Fe_{0.1}Mn_{0.9}O_3$ measured at 300 K and Rietveld refinement in the orthorhombic Imma space group.*

Borosilicate glasses. — Alkali borosilicate glasses are of significant current interest as suitable materials for isolating host media for radioactive waste material storage (i.e. UO_3 or PuO_2). In order to get information on the local structure we have performed neutron- and high energy X-ray diffraction experiments on a multi-component borosilicate glass with the actual composition of $55SiO_2 \cdot 10B_2O_3 \cdot 25Na_2O \cdot 5BaO \cdot 5ZrO_2$ added with 30 wt% UO_3. The two experimental structure factors and the corresponding total atomic

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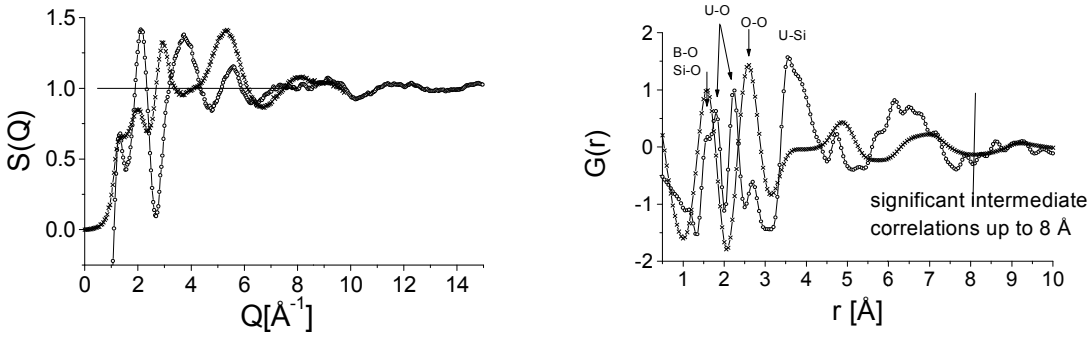
distribution functions calculated by Fourier-transformation are illustrated in Fig. 3. X-ray diffraction data are dominated by contributions from heavier elements (*Ba, Zr, U)*, while neutron diffraction gives information mainly on the light elements (*B*, *O, Si)*. The experimental data were subjected to Reverse Monte Carlo (RMC) modelling. From the atomic configurations several characteristic features of the local order around uranium ion have been revealed. The U-O distribution shows two well resolved peaks centered at 1.8 Å and 2.2 Å, and significant U-Si correlations are present, suggesting that the uranium ions take part in the network forming.



a) *b)*

Fig. 3 *70wt%(55SiO_2·10B_2O_3·25Na_2O·5BaO·5ZrO_2)+30wt%UO_3 glass measured by neutron diffraction (crosses) and hard X-ray diffraction (open circle) a) Structure factors b) Total radial distribution functions.*

Chalcogenide glasses. — $(As_{0.4}S_{0.6})_{100-x}Ag_x$ glasses (x = 0, 4, 8, 12 at.%) have been studied by high-energy x-ray diffraction, neutron diffraction and extended X-ray absorption spectroscopy at As and Ag K-edges. The experimental data were modelled simultaneously by the reverse Monte Carlo simulation method. Analysis of the partial pair correlation functions and coordination numbers extracted from the model atomic configurations revealed that silver preferentially bonds to sulfur in the As_2S_3–Ag ternary glasses, which results in the formation of homoatomic As–As bonds. Upon the addition of Ag, a small proportion of Ag–As bonds ($N_{AgAs} \approx 0.3$) are formed in all three ternary compositions, while the direct Ag–Ag bonds ($N_{AgAg} \approx 0.4$) appear only in the glass with the highest Ag content (12 at.%). Similar to binary As_2S_3, the mean coordination number of arsenic is close to three, and that of sulfur is close to two, in the As_2S_3–Ag ternary glasses. The latter observation strongly suggests that - unlike in As_2Se_3-Ag and As_2Te_3-Ag glasses - Ag is built in the covalent network, which results in a significantly lower mobility of Ag ions.

The structure of $As_3Se_5Te_2$ infrared optical glass was investigated by X-ray and neutron diffraction as well as extended X-ray absorption fine structure measurements at the As-, Se- and Te K-edges. The five datasets were modelled simultaneously by the reverse Monte Carlo simulation technique. Experimental data could be fitted satisfactorily by allowing As–Se, As–Te and Se–Te bonds only. It was revealed that the affinity of As is much higher to Se than to Te. The nearest As–Se distance is similar to that found in other vitreous As–Se based alloys, while the As–Te bond length is 0.02–0.04 Å shorter in $As_3Se_5Te_2$ than in binary As–Te glasses.

Liquids. — Neutron and X-ray weighted total scattering structure factors of liquid carbon, silicon, germanium and tin tetrachlorides, CCl_4, $SiCl_4$, $GeCl_4$ and $SnCl_4$, have been 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. Via comparison with reference systems, obtained by hard sphere Monte Carlo simulations, we demonstrated that orientational correlations characterizing these liquids are much longer ranged than expected, particularly in carbon tetrachloride.

A detailed study of the microscopic structure of an electrolyte solution, cesium chloride (CsCl) in water, was carried out. For revealing the influence of salt concentration on the structure, CsCl solutions at concentrations of 1.5, 7.5 and 15 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. This combination of computer modeling methods is capable of (a) showing the extent to which simulation results are consistent with experimental diffraction data and (b) tracking down distribution functions in computer simulation that are the least comfortable with diffraction data. For the present solutions we show that the level of consistency between simulations that use simple pair potentials and experimental structure factors is nearly quantitative. Remaining inconsistencies seem to be caused by water-water distribution functions. From the particle coordinates, provided by RMC, distribution of the number of first neighbors, as well as angular correlation functions were calculated. The average number of water molecules around cations decreases from about 8 to about 6.5 as concentration increases from 1.5 molar % to 15 molar %, whereas the same quantity for the anions changes from about 7 to about 5. It was also found that the average angle of Cl…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). The present combination of experimental and computer simulation methods appears to be promising for the study other electrolyte solutions.

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Grants and international cooperations

OTKA T 048580 Structural studies of liquids and amorphous materials by diffraction and computer modelling (L. Pusztai, 2005-2009)

MTA-BAS (Hungarian-Bulgarian bilateral): Neutron scattering investigation of the structure of ordered and disordered magnetic and non magnetic materials (E. Sváb, 2007-2009)

MTA-BAS (Hungarian-Bulgarian bilateral): Study of the structure and optical properties of multicomponent chalcogenide materials (E. Sváb, 2007-2009)

MTA-CONACyT (Hungarian-Mexican bilateral): Towards the understanding of the microscopic structure of aqueous electrolyte solutions: a combined experimental, computer simulation and theoretical approach (L. Pusztai, 2007-2009)

TéT SI-18/2007 (Hungarian-Slovenian bilateral) Structural studies of complex liquids (L. Pusztai, 2008-2009)

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)

Long term visitors

— A. Vrhovšek, University of Ljubljana (1 February – 31 May 2009; host: L. Pusztai)

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L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

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

Experimental research. — We performed several femtosecond technology related investigations on our unique, long-cavity Ti:sapphire oscillator (Fig. 1) which delivers orders of magnitude more pulse energy than standard, short-cavity Ti:sapphire systems. We tested so-called highly dispersive mirrors in the cavity (providing two orders of magnitude more dispersion than standard chirped mirrors) for the first time. In addition, we demonstrated that the pulse energy can be increased from 200 to 500 nJ by acousto-optic cavity dumping of the oscillator (Fig. 1).

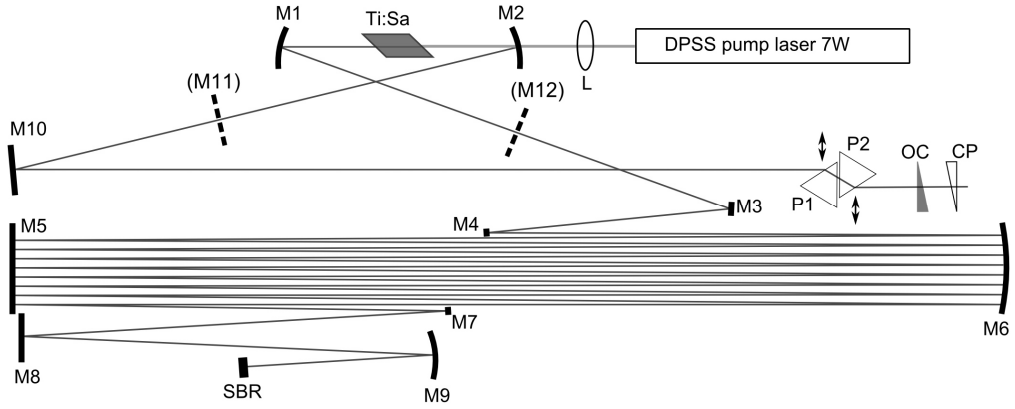

Fig. 1 *Scheme of the long-cavity Ti:sapphire oscillator delivering 40-fs, 200-nJ pulses with a repetition rate of 3.6 MHz.*

We continued the investigation of surface plasmon enhanced electron acceleration induced by few-cycle laser pulses. 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 femtoseconds in the accelerating field).

The STM based laboratory, presented to us by the Max Planck Institute for Quantum Optics has been transferred and put into operation in our laboratory. With the study of the temporal behaviour of STM signals at gold surfaces, the exploitation of this device has been started.

Theoretical research. — The spontaneous emission of metallic electrons embedded in a high-intensity enhanced surface plasmon field has been considered analytically. The electrons have been described by dressed quantum states which contain the interaction with the plasmon field non-perturbatively. Considerable deviations from the perturbative behaviour have been found in the intensity dependence of the emitted fundamental and the second harmonic signals, even at moderate incoming laser intensities. The theoretical predictions deduced from the formalism are in good qualitative agreement with the experimental results.

The familiar 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 initial-value problem of the Schrödinger equation has been solved non-perturbatively for the system of a free electron interacting with a quantized mode of the electromagnetic radiation. Wave packets of the dressed states so obtained have been constructed in order to describe the spatio-temporal separation of the subsystems before and after the interaction. The joint probability amplitudes have been calculated for the detection of the electron at some space-time location and the detection of a definite number of photons. The study of the time evolution of entanglement between the initially separated electron wave packet and the radiation mode led to the conclusion that in general there are non-vanishing entropy remnants in the subsystems after the interaction. On the basis of the simple model discussed, the calculated values of the entropy remnants crucially depend on the character of the assumed switching –on and –off of the interaction, and explicitly reflect back the irreversible character of the process.

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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, 2008-2011)

OTKA F60256 Investigation of femto- and attosecond light-solid interactions with controlled-waveform laser pulses (P. Dombi, 2006-2009)

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), 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, Gy. Farkas)

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

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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, K. Kutasi, P. Mezei

Computational and experimental plasma studies. — In the field of strongly coupled plasma research we have compared microscopic density and current fluctuation spectra for single- and double layered, and three-dimensional Coulomb and Yukawa systems with special emphasis on the higher harmonics generation. We have found second harmonics generation in single component systems and even higher (up to 4^{th} order) harmonics in bilayer systems accompanied by a parity rule for the appearance of the high harmonics in the in- and out-of-phase oscillation modes. With our custom designed and built complex (dusty) plasma experimental facility we have realized a strongly coupled bilayer system of electrically charged spherical dust particles using melamine-formaldehyde microspheres with two different sizes. Our particle-image-velocimetry analysis of the experimental recordings revealed the oscillation mode spectrum unambiguously supporting the predictions of the quasilocalised-charge-approximation theory of the presence of an optic out-of-phase oscillation mode with a finite energy gap at zero wave-number. In the field of the physics of low-pressure gas discharges we have focused our research on numerical simulations of discharges simultaneously excited by two radiofrequency sources. Under such conditions a nearly independent control of the ion energy and the ion flux reaching the electrodes can be realized, which is highly important in plasma processing applications. The computational results have been compared with theoretical as well as experimental results of collaborating partners at the Ruhr University Bochum. Using Monte Carlo type simulation of the electrons' motion we have investigated the electron kinetics under the conditions of the Earth's atmosphere as well as in afterglow plasmas used for the studies of atomic physics processes.

Electrolyte cathode atmospheric pressure glow discharge (ELCAD). — The ELCAD operates in the saturated water vapor, hence the correct determination of the T_G gas temperature is based on the intensity ratio of the ultraviolet band heads of OH radicals. The T_e electron temperature was received from the measured intensity ratio of the Cu-I 510.5 and 515.3 nm lines. Due to the atmospheric pressure, $T_e \approx T_G$. The intensity distribution of the N_2-337 nm band measured along the central, vertical axis of the discharge referred to that N_2 is present only in the outer shell of the plasma.

The radial intensity distributions of the N_2-337 nm and OH-306 nm bands were determined by digital image processing. The total picture of the ELCAD-plasma was imaged to a HAMAMATSU S7010 UV sensitive CCD camera, so that the corresponding 337 nm or 306 nm filter was placed before the CCD camera. At two different distances from the cathode, an Abel-inversion of measured data was performed after a deconvolution calculation. The radial emissivity distributions clearly show the fact that the entering components of the gas atmosphere into the core of the plasma is hindered while OH is a principal component there. Since N_2 is mostly present in the outer shell of discharge, where the rate of excitation is much lower than that inside of the plasma, the value of T_G obtained from the emitted N_2 bands, is significantly lower compared to that determined from the intensity ratio of the ultraviolet band heads of OH radicals.

Microwave discharge systems for plasma sterilization and nanotechnology. – Surfatron generated surface wave microwave discharges produced in small diameter tubes

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contain high density of active species. When the discharge is created in flowing gas the active species can be transported into an electric-field free large volume reactor that can be used for different applications, such as sterilization of medical tools, deposition of oxide films or oxide nanowires. The main role in these applications is played by the O-atoms. Therefore, we have investigated the evolution of O-atoms densities in Ar-O_2 microwave discharges and post-discharges as a function of different parameters by means of modelling. The surface wave microwave discharge is described by a zero-dimensional kinetic model, while the density distributions in the post-discharge reactor are determined with a 3-D hydrodynamic model. The UV photons present in these systems are also useful since they can be responsible for the deactivation of different bacteria. The densities of UV emitting species in Ar-O_2, Ar-O_2-N_2 and N_2-O_2 have been calculated in the discharge zone and in the post-discharge reactor. Further, the intensity of UV emission at different discharge conditions and system configurations has been estimated.

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Grants and international cooperations

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

OTKA K-68390 Investigations of the atomization processes in the electrolyte cathode atmospheric glow discharge (P. Mezei, 2007-2011)

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

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)

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N. LASER APPLICATION

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

The success story of this year is the winning of the site choice competition within the **Extreme Light Infrastructure (ELI) ESFRI Projects** together with Czech Republic and Romania. The Hungarian participation is co-ordinated by our Institute. Thirteen European countries participate in this project and 5 of them applied for hosting the infrastructure facility. According to the declaration of the Steering Committee from the 1st of October, 2009, the Attosecond Infrastructure facility will be built in Hungary.

This will be the first infrastructure dedicated to the fundamental study of laser-matter interaction in a new ultra-relativistic regime of light intensity. It would be a unique laser operating at ~ 100PW level and at the centre of the beam ~1000 times more powerful than other lasers worldwide. In contrast to other projects, ELI would attain its extreme power from the shortness of its pulses. This will give us the possibility to study ultrafast processes of molecules to quarks at the attosecond timescale. A recent revolution in laser technology has opened the door to the generation of flashes of light that can freeze the ultrafast motion of electrons inside atoms and molecules. This infrastructure would serve to build and investigate a new generation of compact accelerators delivering energetic particle and radiation beams of femtosecond (10^{-15}s) to attosecond (10^{-18}s) duration. Relativistic compression offers the potential of intensities exceeding IL>10^{25} W/cm², which would challenge the vacuum critical field as well as provide a new avenue to ultrafast attosecond to zeptosecond (10^{-21}s) studies of laser-matter interaction. ELI would offer wide benefits to society ranging from improvement of oncology treatment, medical imaging, fast electronics and our understanding of aging nuclear reactor materials to development of new methods of nuclear waste processing.

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 Meetings and Steering Committee Meetings (the WP4 meeting and Steering Committee Meeting were organised in Budapest) we made a dozen of presentations and discussed our possible involvement and responsibilities in different tasks to be developed and a number of experimental applications. So we will take care of the development of interferometric and light scattering methods for testing of optical elements of the laser system (e.g. surface testing with nanometer resolution), vibration analysis and alignment control, investigation of the optical quality of the substrates and crystals using high dynamic range light scattering, development and production of special optical coatings (AR, beam splitters, mirrors, etc.), development of special metrologic equipment to measure statistical parameters etc.

Optical measuring techniques. — This year we tested the portable industrial version of the dual wavelength optical particle analyzer enabling simultaneous measurement of the concentration, size distribution, refractive index and absorption of the aerosol particles which was developed last year. This instrument is controlled by a laptop PC, but has also a built-in control panel. The device was installed in a mobile laboratory – in a minivan and was implemented in 2 measurement campaigns and a number of different measurements in different places.

[#] Ph.D. student

During these campaigns, the atmospheric aerosols and toxic gases in different locations during different seasons of the year were measured. In one of these campaigns - air contamination maps of Budapest airport and its surrounding were composed. The measured parameters can help us to determine the origin of the measured aerosol contamination and give more complete information about the particles as any existing device in this field. The other benefit of the developed devices is the possibility to perform the measurements with short sampling time (~ 1 s), without considerable dead time, so even fast changing of the atmospheric pollution can be registered. The sensitivity and resolution of the device was also increased.

The aerosol particle deposition in human airways was modelled and specific deposition parameters were determined in case of diseased airways.

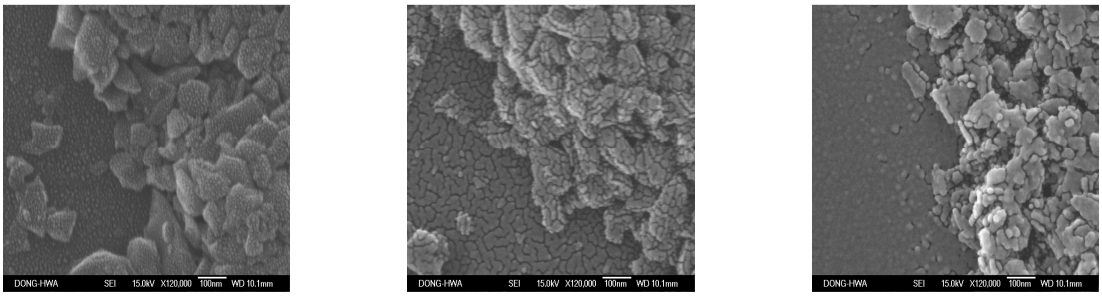
Measurement of the statistics of photons generated in different nonlinear optical processes were performed. The surface plasmon (SP) generation and its statistical properties were studied. The statistics of the excitation light and the light generated by surface plasmons was compared. The temporal statistical behaviour at low excitation level, as measured by detecting the SP emitted photon statistics as expressed by the correlation function and the temporal photon count distribution, show that the SP generated light preserve the photon statistics of the exiting laser.

A 3 year development project has been started as well, under the financial support of KMOP-1.1.1-07/1-2008-0056 project. The aim of this project is the construction of a new nanoparticle velocity and size measuring instrument for serial production. The lower size limit for particles with moderate refractive index is in the range of 50 – 500 nm. The prototype of this serial product was constructed this year. Applying backscattering geometry, an illumination optical system and high numerical aperture data collection optics with common optical axis were constructed. Measurement data collection hardware was constructed for operation on four independent channels having user defined analog or ECL (emitter-coupled logic) input. For control of the instrument a measurement and data collection software was developed. Cold testing, calibration, implementation of opto-mechanical unit and measurement data collection hardware and software are successfully performed.

Amorphous carbon layers. — Continuing the detailed study of surface-enhanced Raman scattering of nanocrystalline diamond (NCD) films using gold nanoparticles, an interesting question has arisen namely whether this system could be used for catalysis of CO oxidation or not. For a long time gold was deemed as catalytically inactive material. It was found, however, that in form of small clusters or nanoparticles gold can catalyse many reactions, for instance the low temperature oxidation of CO, and it could be a promising material for advanced harmful gas neutralizing applications and environmental protection. In spite of the numerous investigations the details of the catalytic phenomenon on gold are still not clear. The main problem is the complexity of the preparation methods and the large number of external factors effecting on the catalysis. Therefore a relatively simple, well-controllable method for the preparation of supported Au catalyst would help in better understanding different processes involved in Au catalysis and its broader utilization.

Commercially available nanocrystalline diamond particles having average size of 100 nm were positioned on Si surface by laser acceleration technique and covered with sputtered gold. By increasing the Au deposition time metal layers of different type and thickness were prepared, ranging from island type structures to continuous film (Fig. 1). Chemical species formed under the oxidation process performed in ambient air were analysed by

micro-Raman and FTIR spectroscopy and the results in the interesting wave number region are shown in Fig. 2.



(a) *(b)* *(c)*

Fig. 1 *SEM pictures of gold covered NCD particles prepared with sputtering times of (a) 10 s, (b) 40 s and (c) 90 s. The morphology of the Au coating evolves from separate nanoparticles to a continuous film.*

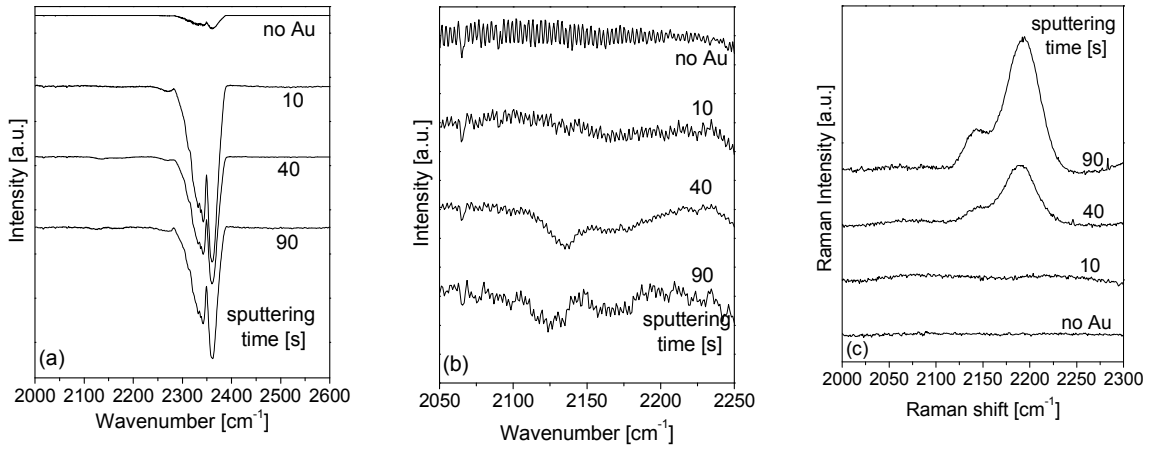


Fig 2 *FTIR spectra of Au-coated NCD samples in the wave number region of (a) CO_2 and (b) CO (enlarged) vibrations. (c) Near-infrared excited Raman spectra of Au-coated NCD crystallites prepared with different sputtering times.*

Comparison of the FTIR spectra of the gold-coated NCD samples with the sample without Au in the CO_2 absorption region exhibits a more than ten times increase in the intensity for the Au-NCD samples (Fig. 2a), indicating the presence of higher amount of CO_2, which cannot arise neither from the air (the contribution of CO_2 molecules of the air was compensated by the background spectrum), nor from the molecules adsorbed on the NCD surface (their contribution is counted in the spectrum of the pristine NCD sample too), but it is definitely related to the presence of Au. Characteristic absorption peaks of Au-based catalysts promoting CO oxidation were also observed in the FTIR spectra (their assignment is given in Table 1). The presence of the above peaks in the FTIR spectra of the Au-NCD samples indicates the catalytic activity of the system, so the nanodiamond can serve as a support for Au catalysts.

Peak position, cm^{-1}	Activity	Assignment
2116	IR	Au^0-CO
2127	IR	Au^0-CO
2137	IR	(Au-O)-CO
2160	IR	Au^{1+}-CO
2180	IR	Au^{1+}-CO

Table 1 *Assignment of the characteristic peaks observed in the FTIR spectra of the sputtered gold coated NCD samples.*

From a further analysis of the Au-NCD samples spectra (Fig. 2a and Fig. 2b) it is seen that the highest intensity of CO_2 peaks appears for the sample having lowest intensity of bands related to adsorbed CO molecules, indicating that the type of aggregation of CO molecules on the gold surface effects on the catalytic activity. Samples with Au^{1+}-CO and some Au^0-CO groups on the surface have lower efficiency. Probably a part of CO molecules occupy the active sites of the catalyst and lower the catalytic activity of the system. Formation of such fragments was also supported by Raman spectroscopic measurements (Fig. 2c), where characteristic peaks of CO chemisorbed to Au^0 surface was observed at 2143 cm^{-1} and 2189 cm^{-1}.

Raman and photoluminescence spectroscopy are powerful methods for the investigation of minerals. These experimental techniques were used to study the miocene hydrothermal bio-mineralization in cryptocrystalline silica varieties, as well as in the Jurassic Fe-Mn oxide rocks forming chimney systems. Disordered carbon phases were found in these rocks, and the parameters of the D and G Raman peaks showed the presence of ring-like structural units evidencing the microbial activity in the mineral. These rocks exhibit intensive light emission under optical excitation which effect supply also information about the bio-mineralization process. Applying luminescence excitation and emission spectroscopy of the above mentioned rocks the broad photoluminescence band was deconvoluted into characteristic fluorescence peaks of well-known phases of the rocks and it was confirmed that an amorphous carbonaceous phase of microbial origin contributes also to the broad fluorescence band.

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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 velocity and size measurement instrument (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)

212105/ELI EU FP7 ESFRI, Extreme Light Infrastructure, co-ordination of Hungarian participation (A. Czitrovszky, 2007-2010)

Bilateral Austro-Hungarian Cooperation, Contract No A-20/1 (A. Czitrovszky)

MTA SZFKI-Envi-Tech Ltd. Co-operation Contract (2008)

Long term visitor

— Prof. Mitsa Vladimir, Uzhgorod State University, Uzhgorod, Ukraine, September 6 – October 5, 2009 (host: M. Koós)

Publications

Articles

N.1. Csikvari* P, Somogyi* A, Veres M, Hárs* Gy, Tóth* A; Investigation of the combined effect of argon addition and substrate bias on the growth of ultrananocrystalline diamond layers; *Diamond Rel Mater*; **18**, 1459-1465, 2009

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See also: L.1.

O. FEMTOSECOND LASERS

R. Szipőcs, P. Antal[#], J. Fekete[#], P. Sándor, A. Szigligeti

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

Phase properties of dielectric multilayer mirrors have attracted great interest since we invented chirped mirror (CM) coatings in 1993. We developed these mirrors for intra- or extra-cavity, broadband feedback and dispersion control in femtosecond (fs) pulse solid state laser systems. Dispersion of a chirped mirror structure primarily originates from the frequency dependent penetration depth of the different spectral components. Dispersion compensation by laser mirrors may also rely on resonances built up in the multilayer structure, like in the case of a Gires-Tournois interferometer (GTI) mirror, where a resonance caused by a tiny GTI cavity is responsible for the negative group delay dispersion over a limited bandwidth (typically 1-5% of the central frequency). In contrast to CM-s, the maximum value of group delay on reflection is not limited by the overall optical thickness of the GTI type multilayer coating, hence higher values of the group delay dispersion (GDD) can be obtained over a higher bandwidth (typically 5-15% of the central frequency) with dispersive mirror designs comprising properly tailored, multiple cavities (MCGTI mirrors). Both in chirped mirror structures and GTI-type mirrors, a standing wave field builds up for each spectral components inside the multilayer structure from the incident electromagnetic wave. Below we show that energy stored by the standing wave field determines the phase properties of the dielectric multilayer structures.

We examined different highly reflective (HR) multilayer mirror structures to demonstrate the proportionality of the reflection group delay and the stored energy. We used the well known matrix method to calculate the standing wave electromagnetic field inside the multilayer structure. In all cases, normal incidence of light was assumed and the incident spectral density was wavelength independent. In order to check whether the U/τ_{gr} ratio is independent from the wavelength, we calculated the maximum of this ratio within the HR range ($|r|^2 > 0.997$) and then the relative difference from this maximum:

$$relvar(U/\tau_{gr}) = -\left(\max(U/\tau_{gr}) - U/\tau_{gr}\right)/\max(U/\tau_{gr})$$

We expected that the change of $relvar(U/\tau_{gr})$ is much smaller than unity within the HR region. Among others, we investigated an ultrabroadband chirped mirror (UBCM) design, first we reported in 1997. This kind of UBCM-s are now used for dispersion control and feedback over an octave bandwidth resulting in sub-5-fs laser pulses. For this specific UBCM design, the maximum change in $relvar(U/\tau_{gr})$ is smaller than 0.015.

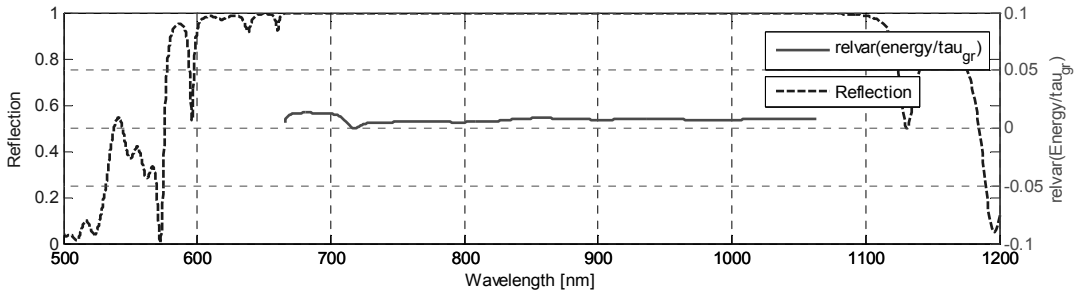

Fig. 1 *UBCM mirror. λ_0 = 790 nm, n_s = 1.51, n_A = 1.00, n_H = 2.315, n_L = 1.45*

[#] Ph.D. student

An other 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. This fact may result in damage threshold problems when they are used in high power laser systems. The maximum change in *relvar*(U/τ_{gr}) is smaller than 0.015.

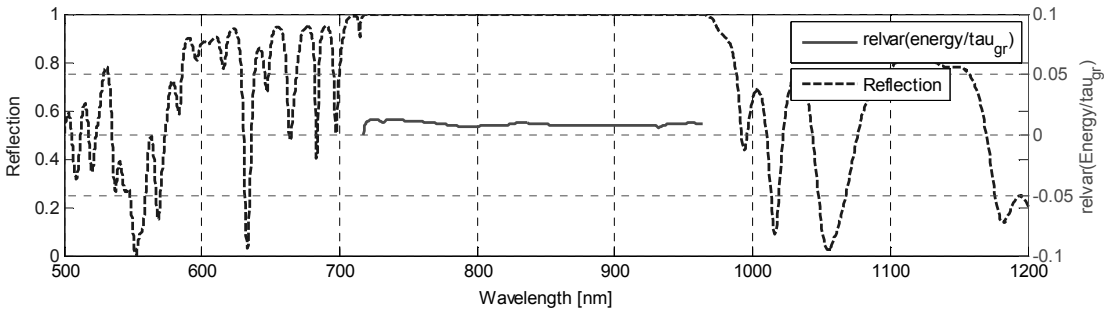

Fig. 2 *MCGTI mirror. λ_0 = 800 nm, n_s = 1.51, n_A = 1.00, n_H = 2.026, n_L = 1.48*

Based on the results listed above, we are convinced that the presented relation between group delay and energy storage in dispersive dielectric mirror coatings leads to a better understanding of dispersive dielectric mirror coatings and to higher performance, more stable optical coating designs.

In 2008, we reported on novel higher-order-mode **solid and hollow core photonic bandgap fibers** exhibiting reversed or zero dispersion slope over tens or hundreds of nanometer bandwidths within the bandgap were developed. This attractive feature makes these devices well suited for broadband dispersion control in femtosecond pulse fiber lasers, amplifiers and optical parametric oscillators. Continuing our research in collaboration with Furukawa Electric Ltd and R&D Ultrafast Lasers Ltd, numerical simulations on different kinds of realistic photonic bandgap fibers exhibiting reversed dispersion slope for the propagating fundamental mode were performed. We found that reversed or flat dispersion functions in a wide wavelength range using hollow-core, air-silica photonic bandgap fibers and solid core Bragg fibers with step-index profile can be obtained by introducing GTI-like resonant structures in the fiber cladding. We evaluated the dispersion and confinement loss profiles of these fibers from the Helmholtz eigenvalue equation and the calculated fiber properties were used to investigate the propagation of chirped femtosecond pulses through serially connected hollow core fiber compressors.

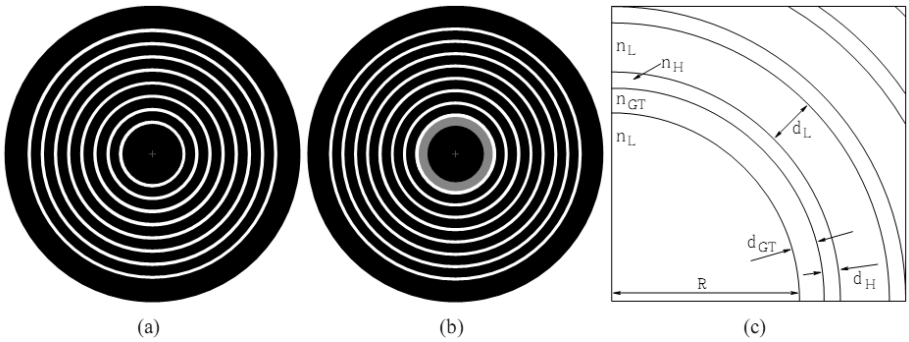

Fig. 3 *(a) SC Bragg fiber with periodic annular layers, (b) SC Bragg fiber with a resonant first layer having a refractive index of n_{GT} and thickness of d_{GT}*

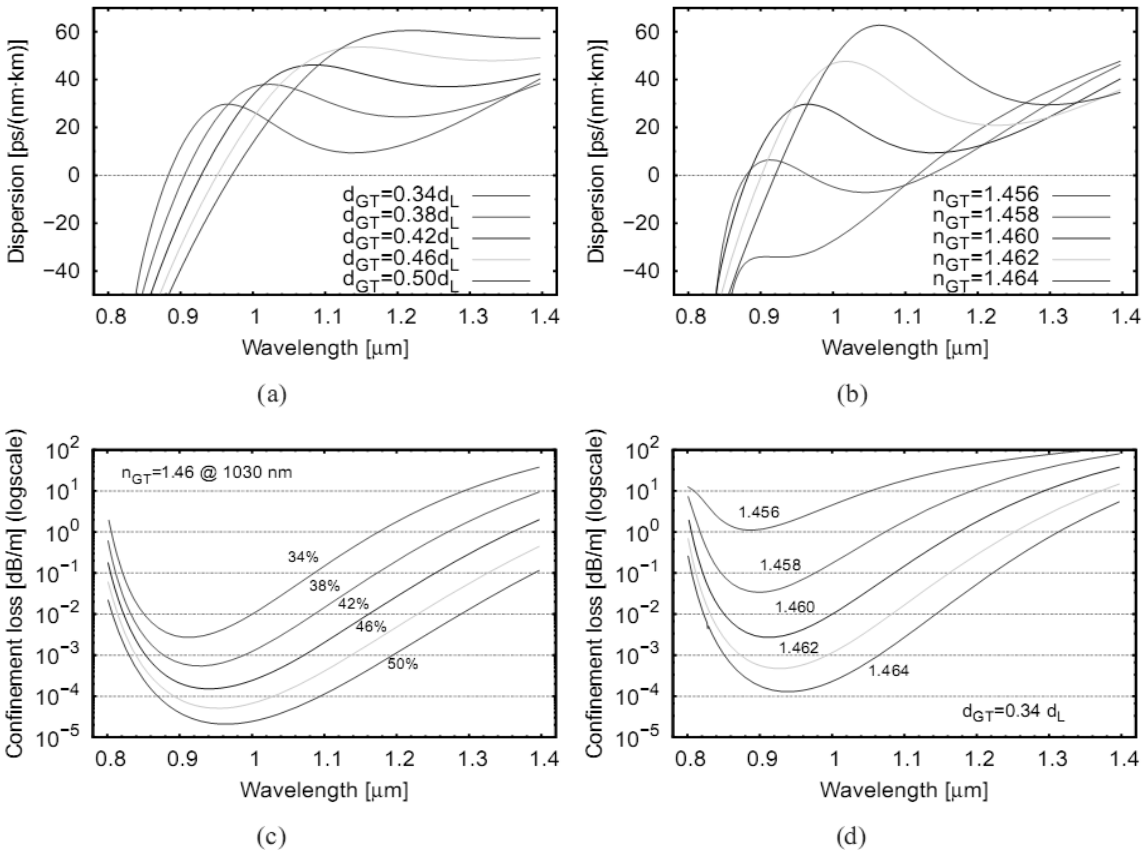

Fig. 4. *Dispersion and confinement loss profiles of different GTIs realized around the core in an SC Bragg PBG fiber. (a) dispersion functions with different thicknesses of GTI, (b) dispersion functions with GTI having different refractive indices, (c) confinement loss belonging to the case changing GTI thicknesses and (d) confinement loss with different GTI refractive indices.*

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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)

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O.6. 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, 2009); accepted for publication

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 silver reflectors (R_p > 98.5%, 400 – 1100 nm, 45°), low dispersion wide-band phase retarding silver mirrors, new type low-dispersion wide-band beam splitter coatings for ultrafast applications for example. Our indium-tin-oxide (ITO) layers having prescribed electrical resistance in the 15 – 35 ohm range were successfully applied as heatable windows in Hungarian military vehicles. Our oxide-free zirconium thin films are used as model materials in the investigation of corrosion processes of nuclear fuel container materials.

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 0.32 nm rms surface roughness on our small size BK7 glass samples superpolished with ceria 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 started new 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) are modifying favourably the colour appearance of the silicon solar cells without decreasing the efficiency because of the coating antireflective effect outside the mirror high-reflectance band.

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. 2815/2009

Grants and international cooperations

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. — A series of rare-earth doped gadolinium aluminum borates (GAB) with the general formula $Eu_xTb_yGd_{1-x-y}Al_3(BO_3)_4$ were prepared by thermal decomposition of the respective metal nitrates, and subsequent solid phase sintering at 950 ^oC in air. Single crystals of GAB:Tb and GAB:Eu,Tb were grown by the high temperature top seeded solution growth (HTSSG) method from a $K_2Mo_3O_{10}$ - B_2O_3 flux. The composition of the crystals was determined by atomic absorption spectroscopy. The crystallographic effect of the Tb and Tb + Eu substitution was investigated by X-ray diffraction via Rietveld refinement of the diffraction patterns. Above a given concentration threshold, the trigonal (R32) structure of GAB has changed to monoclinic (C/2) in the Tb + Eu double doped crystals.

Tm + Yb double-doped yttrium aluminum borate (YAB, $YAl_3(BO_3)_4$) single crystals were grown by the HTSSG method from a $K_2Mo_3O_{10}$ - B_2O_3 flux. The absorption spectrum of the YAB:Tm,Yb crystal was a simple sum of the infrared and visible f—f transitions of Tm^{3+} and Yb^{3+} ions in the YAB crystal field. After excitation at the 975 nm Yb^{3+}-absorption ($^2F_{5/2}$ level), $^3H_4$--$^3H_6$ (803 nm) and $^1G_4$--$^3H_6$ (474 nm) Tm^{3+}-luminescence was observed, reflecting non-resonant energy transfer to Tm-ions and subsequent up-conversion processes. The excitation intensity dependence of the Tm-emission corresponded to 2-photon (for the 803 nm emission) and 3-photon (for the 474 nm emission) processes. After excitation at the 660 nm Tm^{3+}-absorption ($^3F_2$ level) broad, Yb-related emission ($^2F_{5/2}$--$^2F_{7/2}$) was observed in the 950-1070 nm range, reflecting Tm--Yb energy transfer and down-conversion via multiphoton relaxation. The lifetime of the Tm $^3H_4$ (138 μs), $^1G_4$ (100 μs), and Yb $^2F_{5/2}$ (574 μs) levels was determined by short pulse excitation for the Yb 5% + Tm 1% YAB crystal. The radiative lifetimes of the above mentioned excited levels taken from the Judd-Ofelt calculations were 498 μs, 280 μs, and 741 μs, respectively. For the Yb 6% + Tm 3% crystal the experimental lifetimes were shorter due to concentration quenching.

Phase relation of the Li_2O-B_2O_3-Y_2O_3 ternary system has been studied by X-ray phase analysis on ceramic samples synthesized by solid state reaction in the composition range of [Li_2O] = 0,59-0,61 mol%, [B_2O_3] = 0.30-0.31 mol% and [Y_2O_3] = 0.09 - 0.10 mol% in order to determine the concentration region of the crystallization of $Li_6Y(BO_3)_3$ (LYB) phase. By melting the samples, besides the dominant LYB phase, the formation of different stable and metastable compounds (Y_2O_3, $Li_3Y_2(BO_3)_3$, $Li_3Y(BO_3)_2$, Y_3BO_6, YBO_3) have been detected.

The absolute values of effective non-linear optical (NLO) coefficients d_{eff} of β-BaB_2O_4 single crystals were determined by measuring the conversion efficiency of IR and visible light to visible and UV radiation, respectively. The values measured on crystals grown by the Czochralski and the HTSSG methods were compared. No difference in the values of NLO coefficients was obtained for the 1064 to 532 nm conversion, but the d_{eff} values of the crystals grown by the Czochralski method are systematically higher for the 532 to 266 nm conversion.

[#] Ph.D. student

Growth and study of lithium niobate crystals with different compositions and doping. — Pr-doped stoichiometric $LiNbO_3$ crystals were grown by the HTSSG method from K_2O containing flux. The polarized absorption and emission spectra of the Pr^{3+} ion were determined in the 8-300 K temperature range, and were compared to those obtained in Pr-doped congruent crystals. The characteristic f--f transitions and their Stark level structures were similar in these crystals both in absorption and luminescence. However, the sharper peaks in the stoichiometric crystal allowed us to separate the site-selective band components related to different Pr^{3+}-sites in the lattice at low temperatures. The lifetime of the $^1D_2$ level unexpectedly increased from 35.5 to 39.0 μs with increasing temperature (from 10 to 300 K) in the $LiNbO_3$:Pr $2x10^{-3}$ mol% crystal, suggesting limited multiphoton relaxation.

Development of analytical methods for materials science and environmental control. — Graphite furnace atomic absorption spectrometry (GFAAS) method was elaborated and applied to determine Tm-ions in bismuth tellurite crystals. The methodology was optimized for pyrolysis (1150 ^oC) and atomization temperature (2650 ^oC), as well as for chemical modifiers, taking into account the matrix effect of the host crystal. The accuracy of the method was verified by measurements with matrix matched-solution and aqueous standard solutions.

The influence of the modernization of a traffic artery in Mortsel (Antwerp, Belgium) was studied on the atmospheric concentration of volatile organic compounds such as: benzene, toluene, ethylbenzene and m-, p-, o-xylenes (BTEX). The results suggest that the reduction of the number of traffic lanes had apparently increased the traffic jams and also increased the emission from cars, instead of improving the air quality by discouraging the road traffic.

Different ion chromatographic methods were elaborated and tested for separation the F^-, acetate, formate, Cl^-, NO_2^-, Br^-, NO_3^-, HPO_4^{2-} and SO_4^{2-} ions in snow, hail and rainwater samples. The isocratic ion chromatography (IC) with the IC SI-50 4E anion-exchange column using an eluent mixture of 3.2 mM Na_2CO_3 and 1.0 mM $NaHCO_3$ provided the best conditions (shorter than 17 min cycle, 10 ml/min flow).

The chemical composition of airborne particulate matter (PM) and related gaseous pollutants were monitored at the Belgian North Sea coastal region. The daily pollution load was characterized with high levels of fine secondary inorganic aerosols (NH_4^+, NO_3^-, and non-sea-salt SO_4^{2-}) for continental air masses, and sea-salts as the dominant species in coarse maritime aerosols. Increased sea-salt Cl^- depletion was observed in summer (56 %), causing elevated levels of HCl. Neutralization ratios for the coarse fraction (0.6–0.8) suggested a depleted NH_4^+ level, while that for the fine fraction (1.1–1.3) had definitely an excess of NH_4^+, formed by the neutralization of HCl. The results indicated that the major ionic pollutants originated from both local and remote sources.

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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, 2008-2010)

OTKA K-68390 Investigations of atomization processes in an electrolyte cathode atmospheric glow discharge. (P. Mezei, contributor L. Bencs, 2008-2011)

HAS-Polish Academy bilateral cooperation program. Growth and spectroscopic studies of rare-earth doped nonlinear optical crystals. (I. Földvári**,** 2008-2010). Partner: Institute of Low Temperature and Structure Research, PAS, Wroclaw

HAS - CNR bilateral cooperation program. Growth and spectroscopic investigation of self-frequency-doubling laser crystals (I. Földvári, 2007-2009). Partner: Universita di Parma

HAS-Russian Academy of Sciences Project 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 Project 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.

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.

Bilateral cooperation with University of Metz, MOPS, IUT St.-Avold, Common research on non-linear crystals and joint Ph.D. programs (K. Polgár and Á. Péter, 1999-open end)

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Q.3. Buczynska* A, Krata* AA, Stranger* M, Godoi* AFL, Kontozova-Deutsch* V, Bencs L, Naveau* I, Roekens* E, Van Grieken* R; Atmospheric BTEX-concentrations in an area with intensive street traffic in Antwerp, Belgium; *Atmosph Environm*; **43**, 311-318, 2009

Q.4. Dominiak-Dzik* G, Ryba-Romanowski* W, Lisiecki* R, Földvári I, Beregi E; $YAl_3(BO_3)_4$:Yb&Tm nonlinear crystal; up- and down-conversion phenomena and excited state relaxations; *Opt Mater;* **31,** 989-994, 2009

Q.5. Maillard* RS, Maillard* A, Polgár K; Visible and UV non-linear optical coefficients of beta BaB_2O_4 as function of the growth technique; *Opt Mater*; **31**, 899-901, 2009

Q.6. Horemans* B, Krata* A, Buczynska* AJ, Dirtu* AC, Van Meel* K, Van Grieken* R, Bencs L; Major ionic species in size-segregated aerosols and associated gaseous pollutants at a coastal site on the Belgian North Sea; *J Environ Monitor;* **11,** 670-677, 2009

Q.7. Krata* A, Kontozova-Deutsch* V, Bencs L, Deutsch* F, Van Grieken* R; Single-run ion chromatographic separation of inorganic and low-molecular-mass organic anions under isocratic elution: Application to environmental samples; *Talanta;* **79**, 16-21, 2009

Q.8. Bencs L, Krata* A, Horemans* B, Buczyńska* AJ, Dirtu* AC, Godoi* AFL, Godoi* RHM, Potgieter-Vermaak* S, Van Grieken* R; Atmospheric nitrogen fluxes at the Belgian coast: 2004-2006; *Atmosph Environ;* **43,** 3786-3798, 2009

Q.9. Beke* S, Bonse* J, Sugioka* K, Nánai* L, Péter Á, Midorikawa* K; Ablation experiments on TeO_2 crystals in air with femtosecond laser pulses; *J Phys D: Appl Phys;* accepted for publication

Q.10. Van Meel* K, Horemans* B, Krata* A, Bencs L, Buczyńska* AJ, Dirtu* AC, Worobiec* A, Van Grieken* R; Elemental concentrations in aerosols at the Belgian coast versus seasons and air mass trajectories; *Environ Chem Lett;* accepted for publication

Book chapter

Q.11. Bencs L, Ravindra* K, Van Grieken* R; Platinum: Environmental Pollution and Health Effects; In: *Encyclopedia of Environmental Health*; accepted for publication

See also: R.2., R.3., R.4., R.8, R.9., R.10

R. CRYSTAL PHYSICS AND NONLINEAR OPTICS

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

Microscopic studies on imperfections of $YAl_3(BO_3)_4$ (YAB) crystals. — The as-grown surface and inner structures of YAB crystals grown from ($K_2Mo_3O_{10}$ + B_2O_3) flux undoped and doped with various trivalent ions, were investigated using optical and electron microscopic and analytical chemical methods. On the basis of microscopic growth hillocks and oriented straight ribs first observed on the prismatic habit faces of crystals, dislocation densities of about 10^5-10^6 cm^{-2} and the presence of planar microdefects in the increments were detected. In the opaque crystal ranges microinclusions mainly consisting of de- and recomposed constituents from YAB and flux and accumulations of impurity elements, such as Mo, K, Ca, Si, Ti, Na, Mg, and Zn, were revealed by transmission electron diffraction and electron beam microanalysis, respectively. The results give additional information on the formation of grown-in defects in YAB crystals.

Spectroscopy of Eu and Tb doped gadolinium aluminium borate (GAB) crystals. — The concentration, polarization and temperature dependence of the electronic transitions of Eu^{3+} and Tb^{3+} ions were studied by high resolution absorption measurements in GAB crystals in the wavenumber range 2000-34000 cm^{-1}. While the absorption bands of the single doped samples changed only slightly with the rare-earth concentration, splitting and frequency shift of the electronic transitions were observed in the double doped GAB:Eu,Tb crystals as a consequence of the local symmetry changes around the incorporated rare-earth ions. Analysing the temperature dependence of the absorption lines of Tb^{3+} ions, the possible Stark components of the manifolds and the ground state sublevels were identified.

Investigations of $LiNbO_3$ single crystals by transient absorption spectroscopy. — The hitherto unknown absorption cross sections of various kinds of small polarons in $LiNbO_3$ have been determined including hole polarons, free and antisite-trapped electron polarons, and bipolarons formed by the latter two kinds (Fig. 1). Separation of the various contributions could be achieved by comparing transient light-induced absorption changes in the visible and near infrared spectral ranges in various congruent $LiNbO_3$ crystals including undoped samples before and after thermochemical reduction and as grown ones doped by Mg below and above the concentration threshold. These data are crucial for photorefractive and holographic applications.

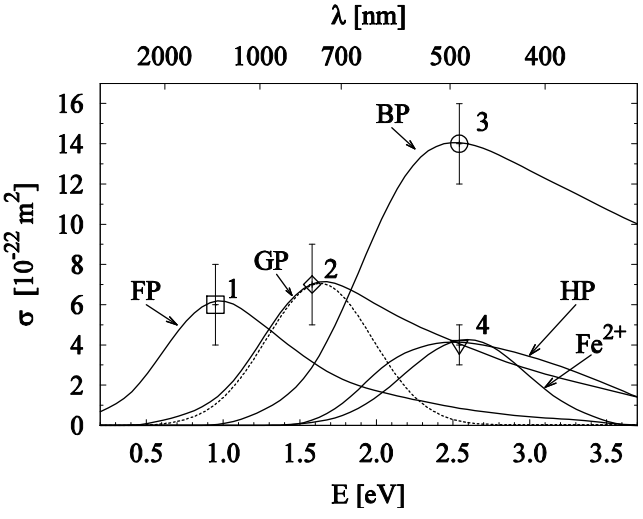

Fig. 1 *Absorption cross sections of small polarons and Fe^{2+} centres in $LiNbO_3$. (HP: hole, FP: free-electron, GP: antisite-bound, BP: bipolaron. The dotted line represents a theoretical polaron band shape for GP.)*

The temperature dependence of the OH vibrational band in stoichiometric $LiNbO_3$ crystal. — The vibrational absorption spectrum of the incorporated OH^- ions in stoichiometric $LiNbO_3$ crystal was studied by high resolution infrared absorption measurements in the temperature range of 8-400 K. The temperature dependence of the frequency of the stretching mode at about 3465 cm^{-1} indicated 3 different coupling phonon modes with wavenumbers at about 73, 314 and 748 cm^{-1}, while in the temperature dependence of the halfwidth only the coupling mode with highest energy appeared.

Coherent radiative processes in $LiNbO_3$:Yb. — High resolution spectral characteristics of a Littrow-type external cavity diode laser to be used for the implementation of coherent radiative processes in $LiNbO_3$:Yb have been determined as functions of temperature, diode current and the piezoelectric voltage of the grating actuator. An optical system has been built for modulating the frequency and amplitude of the laser radiation. The setup involves the near-infrared diode laser at 980 nm, a function generator, a superfine wavelength scanning setup based on an acousto-optical deflector, and a two-channel 200 MHz oscilloscope. A software code has also been developed for the computer control of the measurement.

Spectroscopy of Cu and Ag centres in lithium tetraborate single crystals. — The photoemissions of Cu^+ and Ag^+ centres have been observed in single crystals of the double-doped $Li_2B_4O_7$:Cu,Ag tissue-equivalent thermoluminescent dosimeter and neutron detector material. For UV excitation in the region 6-7eV, enhanced luminescence compared to Cu single doping is due to overlapping emissions of both ions in the region between 3 and 5 eV.

Design and fabrication of diffractive optical elements and waveguides by ion implantation. — The first phase of the design and fabrication of Bragg gratings consisting of multilayers of thin films has been finished. Thin films of SiO_2 were grown by chemical vapour deposition on Si substrate to a uniform thickness of 110 nm, and implanted by 20 keV N^+ and 50 keV Ar^+ ions at doses of 1 x 10^{15} and 1x 10^{16} ions/cm^2, respectively. Part of the samples was thermally annealed at various temperatures. Spectroscopic ellipsometric studies of the ion-implanted thin films confirmed that ion beam implantation resulted in a refractive index change of up to 0.02.

Slab waveguides have been designed and fabricated in CaF_2 crystals and erbium doped tellurite glass samples via implantation of 3.5 MeV N^+ ions at high implanted doses in the range 10^{15} – 10^{17} ions/cm^2. The existence of irradiation-generated colour centres was demonstrated in the ion-implanted CaF_2 samples by absorption spectroscopy. The design of slab waveguides in erbium doped tellurite glass samples using high-energy N^+ ions has been improved by including a second implantation at a slightly lower energy. Results of the simulation of such double-energy implantation using the SRIM 2003 program showed that the implanted barrier layer would be almost twice as thick as that implanted at a single energy. Fabricating waveguides with thick barrier layers would suppress leaky modes even at the telecommunication wavelengths around λ = 1500 nm.

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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, MTA Research Institute for Technical Physics and Materials Science, contributors I. Bányász and A. Watterich, 2007 – 2010)

HAS – Estonian Academy of Sciences joint project: Luminescence and magnetic resonance study of pure and doped wide-gap borate and niobate crystals (G. Corradi, 2007-2009)

HAS – Bulgarian Academy of Sciences joint project: Growth and spectroscopic characterization of oxide crystals for optical application (L. Kovács, 2007-2009)

HAS – CNR joint project: Growth and spectroscopic investigation of self-frequency-doubling laser crystals (I. Földvári, contributors: L. Kovács and K. Lengyel, 2007-2009)

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)

Publications

Articles

R.1. Khanh* NQ, Berneschi* S, Bányász I., Brenci* M, Fried* M, Nunzi Conti* G, Pászti* F, Pelli* S, Righini* GC, Watterich A; Fabrication of channel waveguides in Er^{3+} - doped tellurite glass via N^{+} ion implantation; *Nuclear Instruments and Methods in Physics Research Section B*; **267**, 2327-2330, 2009

R.2. Kovács L, Mazzera* M, Beregi E, Capelletti* R; Infrared absorption spectra of pure and doped $YAl_3(BO_3)_4$ single crystals; *Applied Physics B*; **94**, 273-277, 2009

R.3. Merschjann* C, Schoke* B, Conradi* D, Imlau* M, Corradi G, Polgár K; Absorption cross sections and number densities of electron and hole polarons in congruently melting $LiNbO_3$; *J Phys Condens Matter*; **21,** 015906/1-6, 2009

R.4. Malicskó L, Pogány L, Tóth* AL, Horváth V, Beregi E; Microscopic studies on imperfections in selected YAB single crystals; *Cryst Res Technol*; **44**, 425-432, 2009

Articles in Hungarian

R.5. Hartmann E; Növekedési, egyensúlyi és oldási kristályformák (Growth, equilibrium and dissolution forms of crystals, in Hungarian); *Fizikai Szemle;* **59,** 205-207, 2009

R.6. Hartmann E; BME Kísérleti Fizikai Tanszék 65 éve (65 years of the Department for Experimental Physics of the Technical University in Budapest, in Hungarian); *Fizikai Szemle;* **59,** 278-281, 2009

Conference proceedings

R.7. Berneschi* S, Cacciari* I, Nunzi Conti* G , Pelli* S, Righini* G C, I. Bányász, Khanh* NQ, Lohner* T, Petrik* P, Zolnai* Z, Speghini* A, Bettinelli* M, Mescia* M, Prudenzano* F, Annealing effect on optical barrier in ion-implanted tellurite glass waveguides, In: *Materials, and Technologies XIII, San Jose, CA, USA, 24 - 29 January 2009*; Eds.: Jean-Emmanuel Broquin, Cristoph M. Greiner, Proceedings of SPIE, Bellingham, WA, USA, **218**; p. 721807, 2009

R.8. Schoke* B, Brüning* H, Merschjann* C, Imlau* M, Corradi G, Polgár K, Naumova* I; Transport and recombination behavior of optically generated small polarons with a spatial density modulation in $LiNbO_3$; In: *Topical Meeting Photorefactive Materials, Effects and Devices – Control of Light and Matter, June 11-14, 2009*; Eds: C. Denz and K. Buse, Bad Honnef, Germany; p.108-109, 2009

R.9. Pálfalvi* L, Lengyel K, Péter Á, Fülöp* JA, Reiter* T, Hebling* J; Theoretical and experimental development of the Z-scan method and its application for the characterization of $LiNbO_3$; In: *Proceedings of SPIE, International Conference on Ultrafast and Nonlinear Optics, September 14-18, 2009, Burgas, Bulgaria*; accepted for publication

R.10. Corradi G, Nagirnyi* V, Watterich A, Kotlov* A, Polgár K; Different incorporation of Cu^+ and Cu^{2+} in lithium tetraborate single crystals; *J Phys Conf Series*; accepted for publication

S. QUANTUM OPTICS AND QUANTUM INFORMATICS

P. Ádám, P. Domokos, A. Gábris, J. Janszky, O. Kálmán, A. Kárpáti, Zs. Kis, T. Kiss, M. Koniorczyk, Z. Kurucz, D. Nagy[#], V. Szalay, G. Szirmai, G. Tóth

Laser-induced dynamics of atoms, cavity QED. — We presented a one-dimensional scattering theory which enables us to describe a wealth of effects arising from the coupling of the motional degree of freedom of scatterers to the electromagnetic field. Multiple scattering to all orders is taken into account. The theory was applied to describe the scheme of a Fabry-Perot resonator with one of its mirrors moving. The friction force, as well as the diffusion, acting on the moving mirror is derived. In the limit of a small reflection coefficient, the same model provides for the description of the mechanical effect of light on an atom moving in front of a mirror. This result has been highlighted in Nature Photonics, Vol. 3, page 370 (2009), and in Physics, May 11, (2009).

We showed that quantum fluctuations of a cavity field coupled into the motion of ultracold bosons can be strongly amplified by a mechanism analogous to the Petermann excess noise factor in lasers with unstable cavities. For a Bose-Einstein condensate in a stable optical resonator, the excess noise effect amounts to a significant depletion on long timescales.

Quantum information, entanglement and teleportation. — We studied the separability of permutationally symmetric quantum states. We showed that for bipartite symmetric systems most of the relevant entanglement criteria coincide. However, we provided a method to generate examples of bound entangled states in symmetric systems, for the bipartite and the multipartite case. These states shed some new light on the nature of bound entanglement.

Quantum information processing in semiconductor quantum interference devices. — We presented a mechanism to protect quantum information stored in an ensemble of nuclear spins in a semiconductor quantum dot. When the dot is charged the nuclei interact with the spin of the excess electron through the hyperfine coupling. If this coupling is made off-resonant, it leads to an energy gap between the collective storage states and all other states. We showed that the energy gap protects the quantum memory from local spin-flip and spin-dephasing noise. Effects of nonperfect initial spin polarization and inhomogeneous hyperfine coupling have been discussed.

We proposed a scheme to implement the one-dimensional coined quantum walk with electrons transported through a two-dimensional network of spintronic semiconductor quantum rings. In this scheme the coin degree of freedom is represented by the spin of the electron while the discrete position of the walker corresponds to the label of the rings in one of the spatial directions in the network. We assume the presence of Rashba-type spin-orbit interaction in the rings, the strength of which can be tuned by an external electric field. The geometry of the device, together with the appropriate spin-orbit interaction strengths, ensures the realization of the coin toss, i.e., spin flip and the step operator.

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Grants and international cooperations

OTKA T049234 Quantum optical systems and applications in quantum informatics (J. Janszky, 2005-2009)

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

TéT, Hungarian-Czech Bilateral Intergovernmental S&T Cooperation (CZ-10/2007): Properties of quantum walks and quantum flights (T. Kiss, 2008-2010)

TéT, Hungarian-Austrian Bilateral Intergovernmental S&T Cooperation (AT-3/2007): Quantized motion in an optical resonator (P. Domokos, 2008-2009)

Publications

Articles

S.1. Ádám P, Andreev* VA, Janszky J, Man'ko* MA, Man'ko* OV, Man'ko* VI; Tensor product representation of qubit and its transform under linear-operator action; *J Russ Laser Res*; **30**, 109-121, 2009

S.2. Földi* P, Benedict* M G, Kálmán O, Peeters* F M; Quantum rings with time-dependent spin-orbit coupling: Spintronic Rabi oscillations and conductance properties; *Phys Rev B*; **80**, 165303/1-10, 2009

S.3. Földi* P, Kálmán O, Peeters* F M; Stability of spintronic devices based on quantum ring networks; *Phys Rev B*; **80**, 125324/1-9, 2009

S.4. Gühne* O, Tóth G; Entanglement detection; *Phys Rep*; **474**, 1-75, 2009

S.5. Kálmán O, Kiss T, Földi* P; Quantum walk on the line with quantum rings; *Phys Rev B*; **80**, 035327/1-8, 2009

S.6. Kárpáti A, Ádám P, Janszky J; Quantum operations in probabilistic representation; *Physica Scripta*; **T135**, 014054/1-4, 2009

S.7. Kiss T, Kecskés L, Stefanak* M, Jex* I; Recurrence in coined quantum walks; *Physica Scripta*; **T135**, 014055/1-3, 2009

S.8. Kurucz Z, Sorensen* M W, Taylor* J M, Fleischhauer* M, Lukin* M D; Qubit protection in nuclear-spin quantum dot memories; *Phys Rev Lett*; **103**, 010502/1-4, 2009

S.9. Potocek* V, Gábris A, Kiss T, Jex* I: Optimized quantum random-walk search algorithms on the hypercube; *Phys Rev A*; **79**, 012325/1-6, 2009

S.10. Stefanak* M, Kiss T, Jex* I; Recurrence of biased quantum walks on a line; *New J Phys*; **11**, 043027/1-15, 2009

S.11. Szirmai G, Nagy D, Domokos P; Excess noise depletion of a Bose-Einstein condensate in an optical cavity; *Phys Rev Lett*; **102**, 080401/1-4, 2009

S.12. Tóth G, Wieczorek* W, Krischek* R, Kiesel* N , Michelberger* P, Weinfurter* H; Practical methods for witnessing genuine multi-qubit entanglement in the vicinity of symmetric states; *New J Phys*; **11**, 083002/1-18, 2009

S.13. Tóth G, Gühne* O; Entanglement and permutational symmetry; *Phys Rev Lett*; **102**, 170503/1-4, 2009

S.14. Tóth G, Knapp* C, Gühne* O, Briegel* HJ, Spin squeezing and entanglement; *Phys Rev A*; **79**, 042334/1-13, 2009

S.15. Wieczorek* W, Krischek* R, Kiesel* N, Michelberger* P, Tóth G, Weinfurter* H; Experimental entanglement of a six-photon symmetric Dicke state; *Phys Rev Lett* **103**, 020504/1-4, 2009

S.16. Xuereb* A, Domokos P, Asboth J, Horak* P, Freegarde* T; Scattering theory of cooling and heating in optomechanical systems; *Phys Rev A*; **79**, 053810/1-11, 2009

S.17. 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.18. Bouda* J, Koniorczyk M, Varga* A; Random unitary qubit channels: entropy relations, private quantum channels and non-malleability; *Eur Phys J D*; **53**, 365-372, 2009

S.19. Tóth G, Gühne* O; Separability criteria and entanglement witnesses for symmetric quantum states; *Appl Phys B*, accepted for publication;

Conference proceeding

S.20. Tóth G, Knapp C, Gühne O, and Briegel HJ; Generalized spin squeezing criteria: Entanglement detection with collective measurements; In: *Proceedings of QCMC08, Calgary, Canada; AIP Conf. Proc.,* **1110**; 41, 2009

EDUCATION

Graduate and postgraduate courses, 2009

— Solid-state physics (J. Sólyom, ELTE[2])
— Advanced solid-state physics II. (J. Sólyom, ELTE)
— Completely integrable many body systems (F. Woynarovich, ELTE)
— Statistical physics (F. Iglói , SZTE[3])
— 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 I.-II. (I. Vincze, ELTE)
— Amorphous and crystalline materials (S. Kugler* and T. Kemény, BME[4])
— Calorimetry (T. Kemény, ELTE)
— 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)
— Non-conventional materials (Á. Buka, BME)
— Liquid crystals, their chemistry and chemical physics. (K. Fodor-Csorba)
— Pattern formation in complex systems (Á. Buka and T. Börzsönyi, ELTE)
— Physics of granular materials (J. Kertész*, T. Unger* and T. Börzsönyi, BME)
— Group theory in solid state research (G. Kriza, BME)
— Superconductivity (G. Kriza, BME)
— Geothermobarometry and its applications to petrology (J. Dégi, ELTE)
— Geological applications of thermodynamics (J. Dégi, ELTE)
— Investigation methods in materials science (K. Tompa, BME)
— Application of thermal neutrons for study of condensed matter (L. Cser, ELTE)
— Neutron beam methods in materials science, (L, Rosta, BME)

[2] ELTE = Loránd Eötvös University, Budapest
[3] SZTE = University of Szeged
[4] BME = Budapest University of Technology and Economics

— Neutron scattering in condensed matter (L. Rosta, ME[5])

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

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

— Experimental methods in materials science (M. Veres, BME)

— Classic theories of crystal nucleation (L. Malicskó, BME)

— Theories of crystal growth (L. Malicskó, BME)

— Microscopic characterization of crystals (L. Malicskó, BME)

— Microscopy in materials science (L. Malicskó, BME)

— Technical application of crystals (E. Hartmann, BME)

— The characterization of crystals (E. Hartmann, BME)

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

— Mathematical methods in physics II. (P. Ádám, PTE[6])

— 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)

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

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

— Operating Systems 1. (M. Koniorczyk, PTE)

— Programming 1. (M. Koniorczyk, PTE)

Laboratory practice and seminars

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

— Analysis (R.Juhász, PPKE[7])

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

— Infrared spectroscopy of fullerenes; part of the advanced Molecular Physics Laboratory, K. Kamarás, ELTE)

— Infrared and Raman spectroscopy of solids; part of the advanced Condensed Matter Laboratory (Á. Pekker, Zs. Szekrényes, BME)

[5] ME = University of Miskolc

[6] PTE = University of Pécs

[7] PPKE = Pázmány Péter Catholic University

— Experiments on liquid crystals (Á. Buka and N. Éber, ELTE)

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

— Magnetic resonance techniques (G. Kriza and M. Bokor, BME)

— Laboratory practice on investigation methods in materials science (K. Tompa, BME)

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

— Technical Physics seminar (J.Füzi, PTE)

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

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

— Growth and investigation of periodically poled lithium-niobate and optical characterization of stoichiometric lithium-niobate (Zs. Szaller, G. Dravecz, L. Kovács, ELTE)

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

— Spectroscopic investigation of GAB crystals doped with rare-earth ions (K. Lengyel, ELTE)

— Physics seminar (M. Koniorczyk, PTE)

— Physics Seminar (in English) (M. Koniorczyk, PTE)

— Mathematical programming seminar (M. Koniorczyk, PTE)

Diploma works

D. Varjas (ELTE): Role of Dzaloshinkii-Moriya interaction in pyrochlore lattices in magnetic field (Supervisor: K. Penc)

N. Orsós (SZTE): Application of percolation theory to study entanglement entropy at diluted quantum systems (Supervisor: F. Iglói)

K. Gregó (BME): Structure and thermal stability of fullerene polymers (Supervisor: S. Pekker)

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

A. Bartók (ELTE): Experiments for the preparation of spin-valve structures by electrodeposition (Supervisors: I. Bakonyi and L. Péter)

B.J. Németh (ELTE): Felsic granulite xenoliths from Beistein, Austria: petrography, geochemistry and fluid inclusions (Co-supervisor: J. Dégi)

Á. Tatár (ELTE): Preparation and study of Al-based bulk amorphous-nanocrystalline compacts (Supervisor: L.K. Varga)

P. Simon (BMGE, M.Sc.): Light emission patterns in low pressure glow discharges with small anode electrodes (Supervisor: Z. Donkó)

Á. Varga (PTE): Quantum homogenization and state randomization in semiquantal spin systems (Supervisor: M. Koniorczyk)

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*)

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[8]): 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)

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)

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

É. Fazakas (ELTE): Preparation of bulk amorphous alloys by mechanical alloying (Supervisor: L.K. Varga)

[8] Ecole Polytechnique Fédérale de Lausanne

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*)

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)

Á. Pallinger (ELTE): Dissipation in type-II superconductors (Supervisor: B. Sas)

M. Markó (BME): 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): SANS study of model materials for photosynthesis (Supervisor: L. Rosta)

Zs. Sánta (ELTE): Condensed matter structure investigation with high resolution time-of-flight neutron diffraction (Supervisor: L. Rosta)

N.K. Székely (ELTE): Small angle neutron scattering study of polyol aqueous solutions (Supervisor: L. Rosta)

T. Veres (ELTE): Neutron reflectometry (Supervisor: L. Cser)

A. Len (ELTE): SANS investigation of tungsten wires (Supervisor: L. Rosta)

J. Orbán (BME): Design, implementation and investigation of signal processing electronics for position sensitive particle counters (Supervisors: L. Rosta and Cs. Süközd*)

Sz. Pothoczki (BME): Investigation of the structure of molecular liquids by neutron diffraction and computer simulation (Supervisor: L. Pusztai)

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

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)

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)

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

Ö. Legeza: Application of quantum information theory to strongly correlated systems and the ERA concept. (D. Sc., Hungarian Academy of Sciences)

M. Karsai (PhD, SZTE and University of Grenoble): Cooperative behaviour of complex systems (Supervisor: F. Iglói)

L. Környei (PhD, SZTE): Fractal geometries and their nonequilibrium behaviour in two dimensionak Ising systems (Supervisor: F. Iglói)

M. Fábián (PhD, ELTE): Structure of sodium borosilicate based glasses: neutron diffraction and reverse Monte Carlo modelling (Supervisor: E. Sváb)

S. Tóth (PhD, SZTE): Luminescence and π electronic states of carbon-containing amorphous thin layers (Supervisor: M. Koós)

J. Fekete (PhD, ELTE): Investigation and control of ultrashort pulse propagation in photonic crystal fibers and fiber lasers in the near infrared wavelength region (Supervisor: R. Szipőcs)

G. Dravecz (Ph.D, ELTE and Paul Verlaine University, Metz): Study of the phase equilibria in the ternary systems X_2O Li_2O Nb_2O_5 (X = Na, Rb, Cs), single crystal growth and characterization of $LiNbO_3$ (Supervisors: K. Polgár, M. Ferriol*)

A. Kárpáti (PhD, PTE): Constructive decoherence in quantum systems (Supervisor: P. Ádám)

AWARDS

— N. Kroó, Willis E. Lamb Award for Laser Science and Quantum Optics (2008)

— N. Kroó, Honorary doctor, ELTE

— Ö. Legeza: Bolyai memorial plaquette (2009)

— K. Penc: Physics Prize of the HAS, 2008

— E. Szirmai: Honor of the Hungarian Academy of Sciences for the prominent work as Young Research Fellow, 2008

— Z. Kis: APS Outstanding Referee

— R. Juhász: SZFKI Annual Publication Award (2009)

— T. Balázs: Genius Cup GENIUS-EUROPE International Inventions Fair, Budapest, 2009

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

— P. Jóvári: Bolyai Grant (2008-2011)

— K. Kutasi Young Investigator's prize of the Hungarian Academy of Sciences

— P. Dombi: Bolyai Grant (2007-2010)

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

— K. Kutasi: Bolyai Grant (2008-2011)

— Z. Kis: Bolyai Grant (2007-2010)

MEMBERSHIPS

— N. Kroó: Member of the Scientific Council of the European Research Council

— N. Kroó: Chairman of the Research Infrastructure Expert Group of ERA (EC)

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

— N. Kroó: Member of the Advisory Group on ESOF 2008

— N. Kroó: Member (former Chair) of the Section of Physical and Engineering Sciences of Academia Europaea

— N. Kroó: Member of the Council of the International Council for Science (ICSU)

— N. Kroó: Vice-President of the Hungarian Academy of Sciences

— N. Kroó: Member of the Hungarian UNESCO Committee

— N. Kroó: Chairman of the Committee of International Relations of HAS

— N. Kroó: Member of the Presidium of HAS

— J. Kollár: Chairman of the Committee on Solid State Physics of the HAS

— J. Balogh: Member of the International Board on the Application of the Mössbauer effect, IBAME (2007-2012)

— I. Vincze: Ad-hoc Committee of the Hungarian Parliament on the Research and Innovation (2007-)

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

— G. Faigel: XFEL In-kind Review Committee member

— G. Faigel: XFEL Recruitment Committee member

— G. Faigel: President of Physical Section of HAS

— Á. Buka: Member of the Editorial Board, Electronic-Liquid Crystal Communications

— Á. Buka: Member of the International Advisory Board, International Liquid Crystal Conference

— Á. Buka: Member of the International Advisory Board, Condensed Matter Physics Conference

— Á. Buka: Member of the Presidium of HAS

— Á. Buka: Member of the Council of Academic Institutes

— K. Fodor-Csorba: Member of the ESF COST D35 Management Committee

— K. Fodor-Csorba: Board member of the Open Organic Chemistry Journal

— N. Éber: Member of the International Liquid Crystal Society, Board of Directors

— N. Éber: Member of the Open Crystallography Journal, Editorial Board

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

— I. Bakonyi: Member of the Editorial Advisory Board (2005-), Journal of Materials Science and Technology (Bulgaria, Sofia)

— I. Bakonyi, Member of the Scientific Committee and Advisory Board (2nd Int. Conf. on Functional Nanocoatings, Dresden, 2010)

— I. Bakonyi: Member of the European Board (2006-), European Academy of Surface Technology (EAST)

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

— I. Bakonyi (member) and L. Péter (secretary) of EDNANO Board (2006-), International Workshop on Electrodeposited Nanostructures (EDNANO)

— L. Péter, Editor for Electrochemistry (Central European Journal of Chemistry, 2009-)

— F. Mezei: Scientific Advisory Council of SNS (Spallation Neutron Source), Oak Ridge National Laboratory, USA)

— L. Cser, F. Mezei, L. Rosta: International Scientific Advisory Council of BNC (Budapest Neutron Centre)

— Z. Donkó: Member of the International Scientific Committee of conference series: Symposium of the Phenomena in Ionized Gases

— Z. Donkó: Member of the International Advisory Board of conference series: Strongly Coupled Coulomb Systems

— Z. Donkó: Member of the International Scientific Committee of conference series: Symposium on Application of Plasma Processes

— P. Hartmann: Member of the International Scientific Committee of conference series: Europhyics Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG)

— K. Kutasi: Member of the International Scientific Committee of conference series: International workshop on nonequilibrium processes in plasma physics and studies of environment

— Horváth Z Gy: Vice-Secretary of the Hungarian Medical Laser and Optical Society

— A. Czitrovszky: President of the European Aerosol Assembly (EAA)

— A. Czitrovszky: Chairman of the Working Group Instrumentation in EAA

— A. Czitrovszky: Member of the Board of International Aerosol Association

— A. Czitrovszky: Member of Gesellschaft für Aerosolforschung

— A. Czitrovszky: President of the Hungarian Aerosol Society

— A. Czitrovszky: Member of ELI Participant Council

— A. Czitrovszky: President of the Hungarian Branch of the European Optical Society

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

— A. Czitrovszky, G. Faigel and F. Iglói: Members of the Editorial Board of “Fizikai Szemle”

— A. Czitrovszky: Chairman of the Optical Society of Loránd Eötvös Physical Society

— A. Czitrovszky – Member of the Int. Organizing Committee of European Aerosol Conference (Karlsruhe, 2009)

— A. Czitrovszky – Member of the Int. Organizing Committee of Int. Conf on Advanced Laser Technologies (Antalya, 2009)

— A. Czitrovszky: Chairman of the Committee for the Lasers Physics and Spectroscopy in HAS

— K. Polgár: Hungarian Council Member in the International Organization for Crystal Growth

— L. Bencs: Editorial Board Member of the international journal "Environmental Monitoring and Management"

— L. Kovács: Member of the International Advisory Committee, EURODIM-ICDIM

— L. Kovács: 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

— J. Janszky: Member of the Editorial Board of Problems in Physics

CONFERENCES

— A working group meeting of the **ESF COST D35 WG 13/05** was organized by K. Fodor-Csorba in Stuttgart on 4-6th of April at the University of Stuttgart with 20 participants. In this working group eight European countries (Italy, Czech Republic, Sweden, Austria, United Kingdom, Germany, Russia and Hungary) take part, the coordinator is K. Fodor-Csorba. In this two day meeting each delegate presented a lecture on the physical and chemical properties of bent-core materials.

— The **1st NSF-OTKA Symposium for Complex Fluids** was organized by I. Jánossy in Eger, at 8 – 10 July, 2009. Participants included besides the researchers of the Complex Fluids Department 7 US and 2 Hungarian students and guests from the US, Portugal, Germany and Serbia.

— **4th Reverse Monte Carlo Conference**, 29 September – 03 October, 2009, Budapest; organiser: L. Pusztai. More than 50 participants attended from Europe, the USA and Japan. Talks and posters presented during the meeting have concerned all aspects of Reverse Monte Carlo modelling, from traditional areas such as glassy and liquid structures to new territories like the interpretation of small angle scattering data. Presentations and related works will appear in a RMC Special Issue of the Journal of Physics: Condensed Matter.

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