ANNUAL REPORT

2008

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

Director: Dr. János Kollár

Address: *Budapest XII., Konkoly-Thege M. út 29-33, Hungary*
Letters: H-1525 Budapest, P.O.B. 49
Phone: (36-1-) 392 2212
Fax: (36-1-) 392 2215
E-Mail szfki@szfki.hu

URL: http://www.szfki.hu/

ANNUAL REPORT 2008

Edited by **L. Csillag, G. Konczos, B. Selmeci, I. Tüttő**

Closed on 5th December, 2008

ISSN 1418-4559

Dear Reader,

It is my pleasure to hand over the 15th, 2008 edition of the Annual Report of the Research Institute for Solid State Physics and Optics.

The predecessor of our Institute was founded by the Hungarian Academy of Sciences in 1981 as part of the well known Central Research Institute for Physics. In 1992 the Research Institute for Solid State Physics became independent. In 1998 the Crystal Physics Laboratory of the Hungarian Academy of Sciences joined us as part of the reorganisation and streamlining of the network of research institutes of the Academy. Since then we have been operating as Research Institute for Solid State Physics and Optics.

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. Since January 1, 2007 the Institute has been hosting the campus research library as well.

About 67 % of our funding is provided by the Hungarian Academy of Sciences; the rest originates from a variety of funding agencies via competitive projects. In basic research the Hungarian Scientific Research Fund (OTKA) has a predominant role. We are working on the implementation of several projects in the EU 7th Framework Programme. The Institute has been invited to participate in the preparatory phase of establishing three large-scale facilities, namely the X-Ray Free Electron Laser (XFEL), the Extreme Light Infrastructure (ELI) and the European Spallation Source (ESS).

Our staff of 198 includes 134 scientists. This year we have published more than 215 papers in high quality international journals and conference proceedings showing a steadily high publication activity over the last years. More than half of the publications feature co-authors from foreign countries indicating the essential role of our international research co-operation. The second volume of the textbook “Fundamentals of Physics of Solids,” by Jenő Sólyom (Springer) has also been published this year. The three-volume work will be a comprehensive overview on modern solid state physics.

Achievements of our scientists have been acknowledged by several awards and nominations. Prof. Norbert Kroó has been elected honorary doctor of the Joint Institute for Nuclear Research, Dubna. Géza Konczos has been awarded by the International Prize 2008 of the Slovak Academy of Sciences for his fruitful cooperation with Slovak scientists

in the field of advanced magnetic materials research. Two of our young researchers have received their PhD degree.

It has become a tradition of the Institute to deliver a prize for outstanding publication activity. In 2008 the publication prize has been awarded to Nándor Éber for his papers published on the studies of liquid crystals.

Since the last edition of this Annual Report, the Institute has lost two outstanding former colleagues, Dr. Ivan Kertész (1940-2008) and Dr. Tivadar Tarnóczy (1929-2008). Ivan was the founder of the Department of Laser Application and initiated several projects on the industrial and medical applications of solid state lasers. Tivadar belonged to the first scientific co-workers of the institute beginning his experimental work on magnetism in 1955.

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

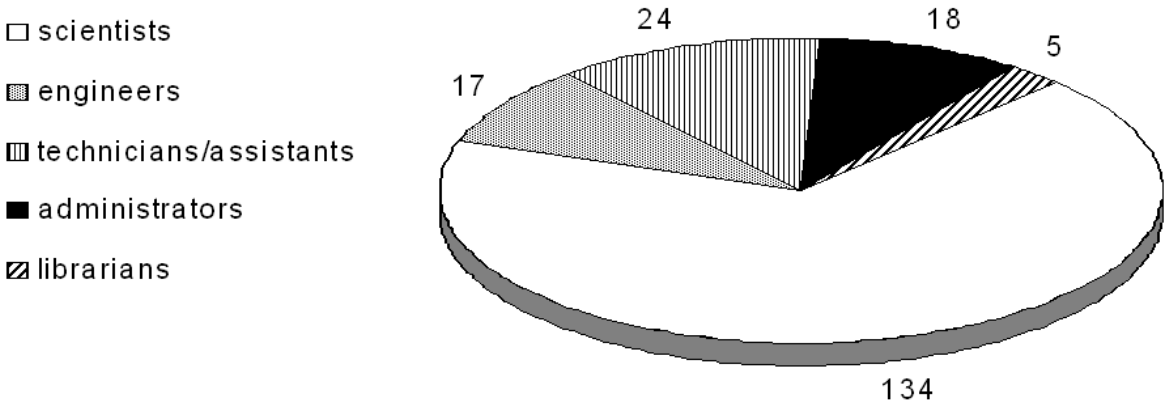
Budapest, December 5, 2008.

János Kollár

Director

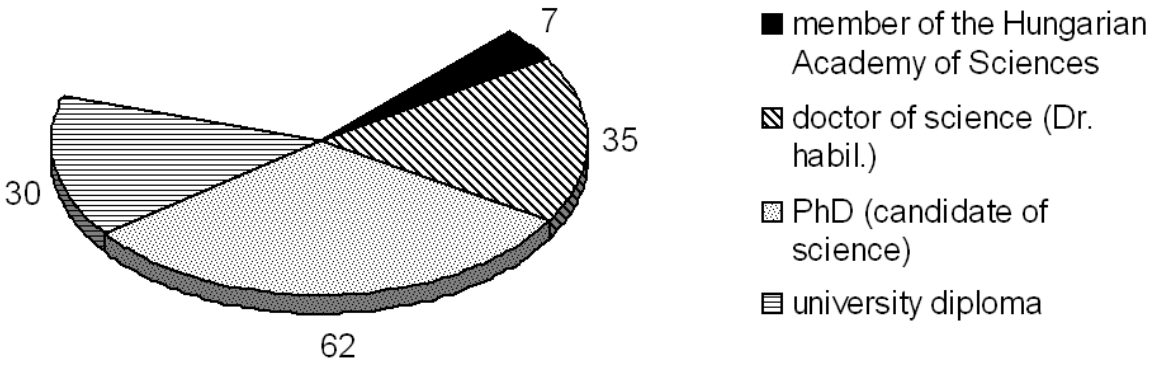
Key figures

Permanent staff of the Institute: 198 employees. Its distribution by professions:

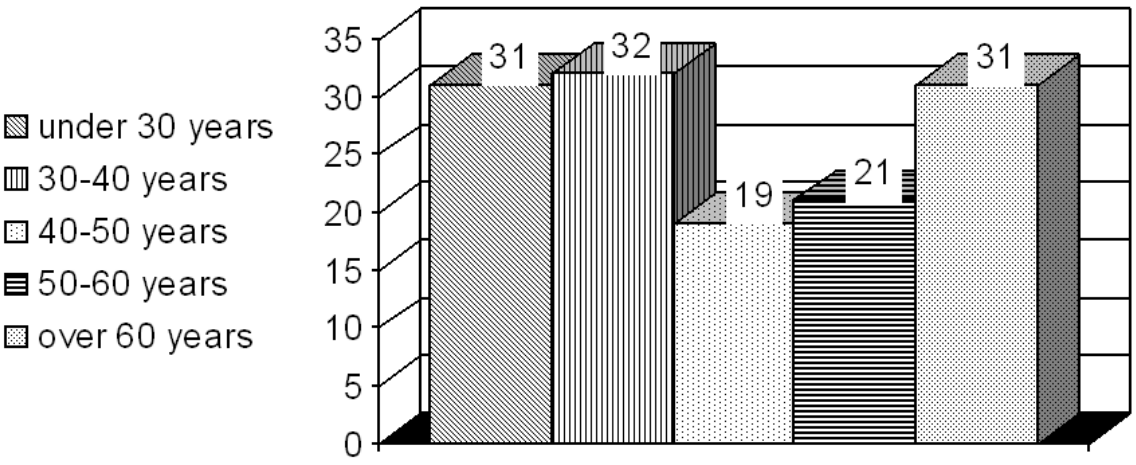


Distribution of scientists:

a) by scientific titles/degrees:

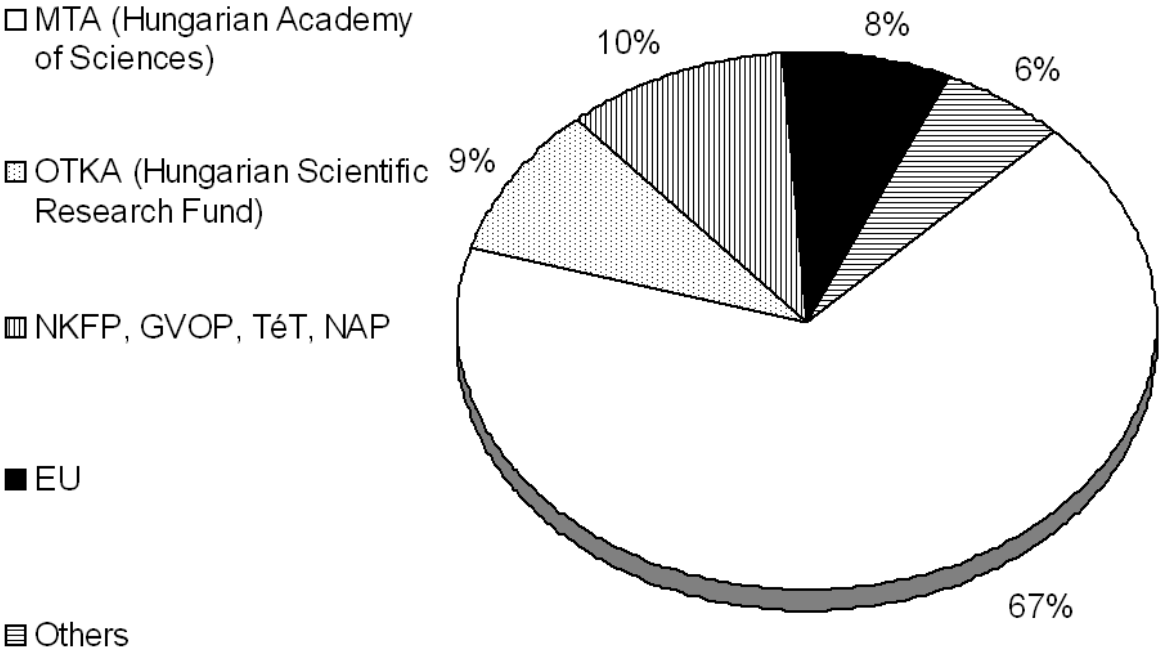


b) by age groups:

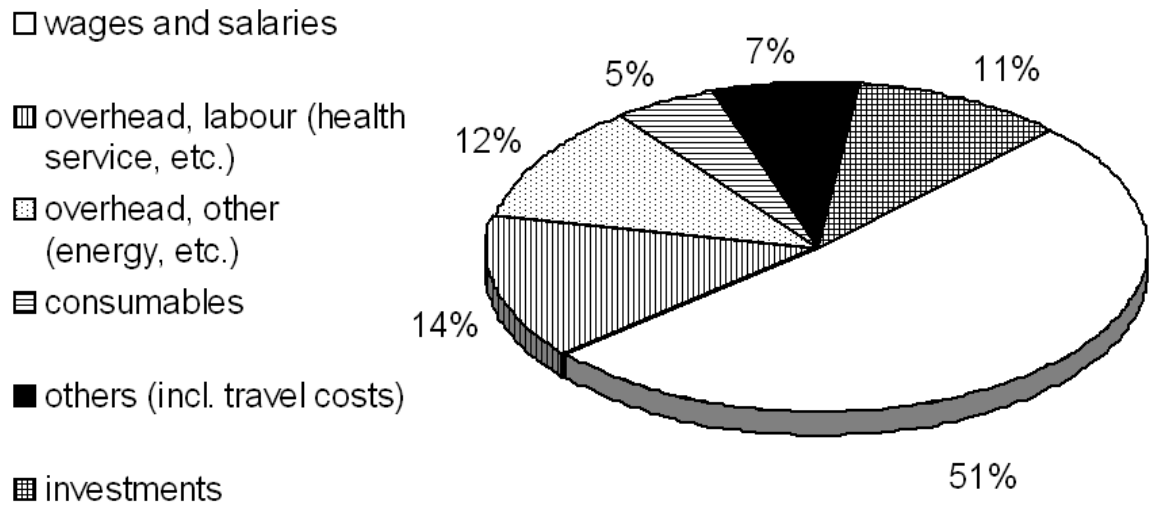


Financial management

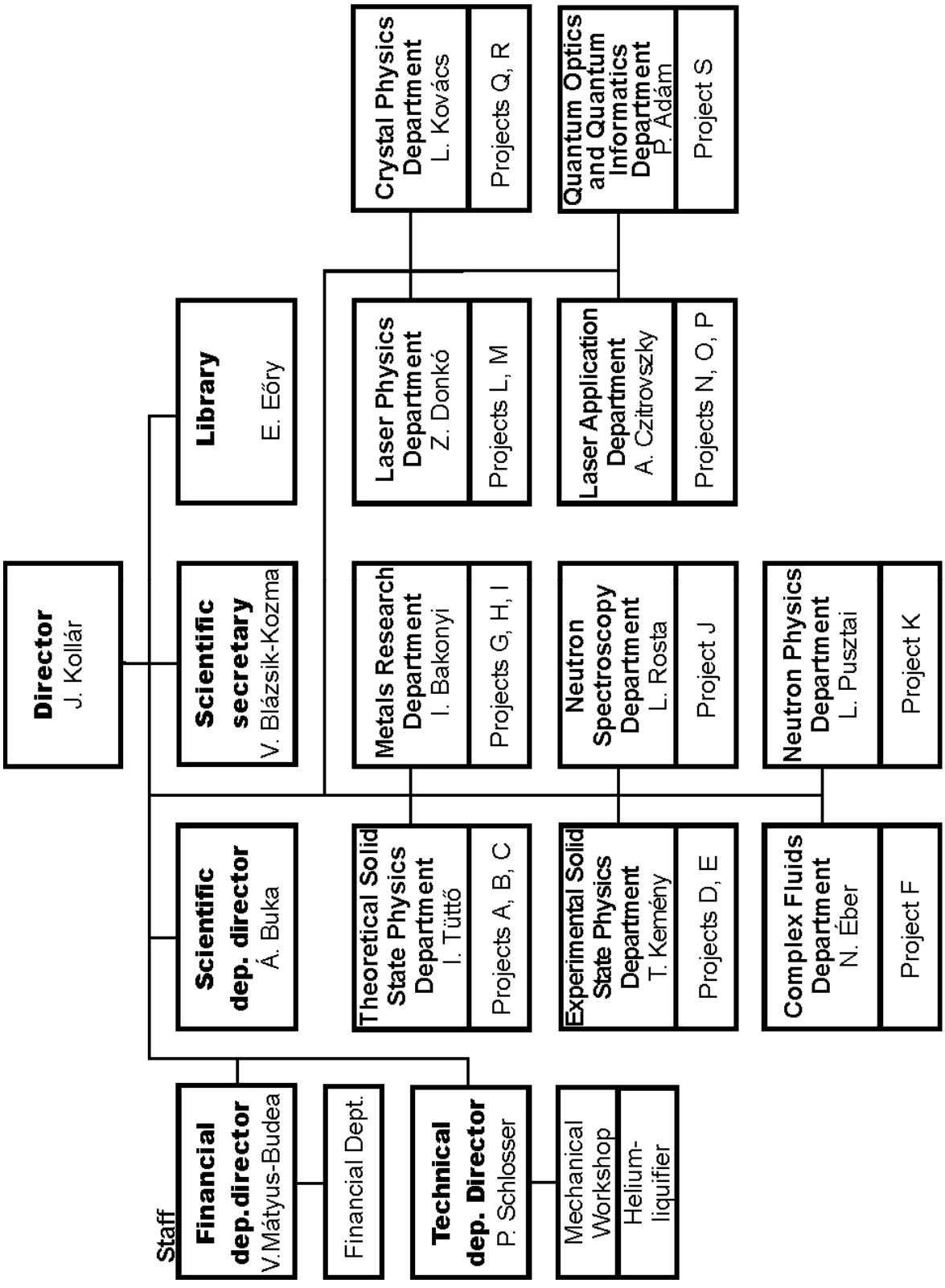
a) Sources of operation costs:



b) Distribution of expenditures:



Structure of the Research Institute for Solid State Physics and Optics



A. STRONGLY CORRELATED SYSTEMS

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

Low-dimensional fermionic models. — We have continued the study of quantum phase transitions by using the density-matrix renormalization-group (DMRG) method. The same models have also been investigated analytically by bosonization.

Ultracold fermionic gases in optical trap can be well described by the Hubbard model and its various extensions. With this in mind we have investigated the role of magnetic frustration in the half-filled extended Hubbard model where nearest- and next-nearest-neighbour spin-exchange with couplings J_1 and J_2, respectively, are also included. In contrast to previous results, the system does not exhibit bond ordering for finite on-site U. The ground state is semi-gapped with dominant spin-density-wave correlations until J_2 is less than a U-dependent critical value. For intermediate values of J_2, especially for strong frustration ($J_1 \sim J_2$), a fully-gapped long-range-ordered phase is stabilized with bond-centered charge-density-wave correlations. Bond ordering is destroyed for large J_2 by charge fluctuations, and a Luther-Emery phase appears.

The SU(n) generalization of the usual SU(2) Hubbard chain was further investigated at commensurate p/q-fillings. Mean-field analysis shows that the bond ordering is a direct consequence of the spin-exchange interaction, which plays a crucial role for intermediate Coulomb repulsion as well.

We have generalized the spectral-sum-rule preserving density-matrix numerical renormalization-group (DM-NRG) method in such a way that it can make use of an arbitrary number of not necessarily Abelian local symmetries present in the quantum impurity system. We have illustrated the benefits of using non-Abelian symmetries by calculating the T-matrix of the two-channel Kondo model in the presence of magnetic field, for which conventional NRG methods produce large errors and/or take a long run-time.

The dynamical correlation functions of one-dimensional electronic systems show power-law behaviour at low energies and momenta close to integer multiples of the charge and spin Fermi momenta. These systems are usually referred to as Tomonaga–Luttinger liquids. However, near well defined lines of the momentum-energy plane the power-law behaviour extends to higher energies, leading to singular features in the photoemission spectra and other dynamical correlation functions. Using the Bethe Ansatz, we systematically enumerate and describe the excitations in the Hubbard model, as well as calculate the phase shifts appearing in the exponents of the correlation functions. We use our results to interpret the photoemission spectra of the quasi-one-dimensional conductor TTF-TCNQ. Our results are useful for the further understanding of the unusual spectral properties observed in low-dimensional organic metals and also provide expressions for the one- and two-atom spectral functions of a correlated quantum system of ultracold fermionic atoms in a 1D optical lattice with on-site two-atom repulsion.

We analyzed the fine structure of excitations in the attractive Hubbard model. We have found a strong collective effect underlying the dependence of energy on the number of

[#] PhD student

[+] Permanent position: Budapest University of Technology and Economics

magnetic excitations that can account for the extremely high, but not divergent susceptibility at the critical point.

Low-dimensional and frustrated magnetic systems. — We have considered topological order and dimer order in several frustrated spin ladder models, which are related to higher dimensional models of current interest; we also addressed the occurrence of fractionalized phases with deconfined spinon excitations in these models. Combining results obtained with both analytic and numerical methods, we have discussed how the occurrence of dimerized or fractionalized phases are dictated by the system's geometry.

Intermediate between single spins and bulk magnets, molecular magnets have attracted a lot of attention since they offer a suitable platform for probing the predictions of quantum mechanics. We have shown that antiferromagnetic rings are unstable towards dimerization at level crossings induced by magnetic field. Unlike the exchange driven spin-Peierls transition of infinite chains, this magnetoelastic instability is triggered by a staggered modulation of the antisymmetric Dzyaloshinsky-Moriya interaction which induces a coupling between the lowest levels and lifts their degeneracy. In agreement with nuclear magnetic resonance and torque experiments reported for the ferric wheel $CsFe_8$, our model accounts for the large staggered transverse polarizations and for the torque anomalies at the level-crossing fields.

E-Mail:

Miklós Lajkó	lajkom@szfki.hu
Örs Legeza	olegeza@szfki.hu
Karlo Penc	penc@szfki.hu
Judit Romhányi	romhanyi@szfki.hu
Jenő Sólyom	solyom@szfki.hu
Edina Szirmai	eszirmai@szfki.hu
Károly Vladár	vk@szfki.hu
FerencWoynarovich	fw@szfki.hu
Alfréd Zawadowski	zawa@phy.bme.hu

Grants

OTKA T049607	Exotic phases and excitation in frustrated electron systems with charge, spin and orbital degrees of freedom (K. Penc, 2005–2008)
OTKA 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. Szirmai E, Legeza Ö, Sólyom J; Spatially nonuniform phases in the one-dimensional SU(*n*) Hubbard model for commensurate fillings; *Phys Rev B*; **77**, 045106/1-10, 2008

A.2. Kim* EH, Legeza Ö, Sólyom J; Topological order, dimerization, and spinon deconfinement in frustrated spin ladders; *Phys Rev B*; **77**, 205121/1-16, 2008

A.3. Huang* X, Szirmai E, Gebhard* F, Sólyom J, Noack* RM; Phase diagram of the *t-U-*J_1*-*J_2 chain at half filling; *Phys Rev B*; **78**, 085128/1-10, 2008

A.4. Carmelo* JMP, Bozi* D, Penc K; Dynamical functions of a 1D correlated quantum liquid; *J Phys Condens Matter*; **20**, 415103/1-17, 2008

A.5. Bozi* D, Carmelo* JMP, Penc K, Sacramento* PD; The TTF finite-energy spectral features in photoemission of TTF-TCNQ: the Hubbard-chain description; *J Phys Condens Matter*; **20**, 022205/1-5, 2008

A.6. Tóth* AI, Moca* CP, Legeza Ö, Zaránd* G; Density matrix numerical renormalization group for non-Abelian symmetries; *Phys. Rev. B*; arXiv:0712.2730, accepted for publication

Conference proceeding

A.7. 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;* arXiv:0805.0982, accepted for publication

Book, book chapter

A.8. Legeza Ö, Noack* RM, Sólyom J, Tincani* L; Applications of Quantum Information in the Density-Matrix Renormalization Group; In: *Lecture Notes in Physics;* **739**, 653-664, Springer-Verlag Berlin Heidelberg (Chapter 24) (2008)

A.9. Sólyom J; Fundamentals of the Physics of Solids, Volume 2 – Electronic Properties, Springer, Berlin Heidelberg, 2008

Other

A.10. Legeza Ö, Moca* CP, Tóth* AI, Weymann* I, Zaránd* G; Manual for the flexible DM-NRG code, Version 1.0.0; arXiv: 0809.3143

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

B. COMPLEX SYSTEMS

F. Iglói, R. Juhász, I. Kovács[#], N. Menyhárd, A. Sütő, Zs. Szép, 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 behavior. — The universality class, even the order of the transition, of the two-dimensional Ising model depends on the range and the symmetry of the interactions (Onsager model, Baxter-Wu model, Turban model, etc.), but the critical temperature is generally the same due to self-duality. Here we consider a sudden change in the form of the interaction and study the nonequilibrium critical dynamical properties of the nearest-neighbor model. The relaxation of the magnetization and the decay of the autocorrelation function are found to display a power law behavior with characteristic exponents that depend on the universality class of the initial state.

We have studied the Ising model on the Bethe lattice with aperiodic modulation of the couplings. We have derived a relevance-irrelevance criterion and solved the critical behavior exactly for marginal aperiodic sequences. We have found analytical formulae for the continuously varying critical exponents and discussed a relationship with the (surface) critical behavior of the aperiodic quantum Ising chain.

We have presented a real space renormalization group scheme for the problem of random walks in a random environment on a strip, which includes the one-dimensional random walk in a random environment with bounded non-nearest-neighbour jumps. We have shown that the model renormalizes to an effective one-dimensional random walk with nearest-neighbour jumps and concluded that Sinai scaling is valid in the recurrent case, while in the sub-linear transient phase, the displacement grows as a power of the time.

The crossover behavior of various one-dimensional parity-conserving models has been investigated by numerical simulations. These models exhibit phase transition into an absorbing phase when an external symmetry breaking field is present. Under the influence of the field the crossover leads to directed percolation kind of behavior. Differing crossover exponents have been found, however, in two classes of models which, in the field-free case, show the same type of (dynamical) critical behaviour. These 'sub-classes' differ in cluster scaling exponents.

Introducing various chemical potentials, the effect of the asymmetric quark matter on the phase diagram of the $SU(3)_L$ X $SU(3)_R$ chiral quark model is investigated. The model is parametrized at one-loop level and solved using the optimized perturbation theory for the resummation of the perturbative series.

A concise method is developed for the non-perturbative renormalisation of a general class of resumed scalar field theories at the Hartree-Fock level truncation of the two-particle-irreducible (2PI) effective action in the broken symmetry regime. The counterterms are explicitly constructed and the method is further extended to λ^2 order in the skeleton truncation of the 2PI effective action of the O(N) model.

Quantum systems. — We have considered two prototypical quantum models, the spin-1/2 XY chain and the quantum Ising chain and studied the entanglement entropy of blocks of contiguous spins in homogeneous and inhomogeneous systems. By using two different approaches, free-fermion techniques and perturbational expansion, we have revealed an

[#] PhD student

exact relationship between the entropies. Using this relation we translate known results between the two models and obtain, among others, the additive constant of the entropy of the critical homogeneous quantum Ising chain and the effective central charge of the random XY chain. We have also studied finite size effects of the entropy at the quantum critical point and studied the scaling behaviour of its maxima, which is used to define an effective critical point in a finite sample.

We have continued the investigations of the trapped Fermi gas, in particular in its superfluid state. Gradient corrections have been determined from the weakly interacting (BCS) limit up to the unitary limit (Feshbach resonance). It has been shown that in such extended local density approximation the superfluid region is located around the center of the trap and its size shrinks when the strength of the interaction decreases.

We studied variational wave functions of the product form, factorizing according to the wave vectors, for the ground state of a system of bosons interacting via positive pair interactions with a positive Fourier transform. Our trial functions were taken from different orthonormal bases in Fock space. Each basis contains a quasiparticle vacuum state and states with an arbitrary finite number of quasiparticles. One of the bases is that of Valatin and Butler (VB), introduced fifty years ago and parametrized by an infinite set of variables determining Bogoliubov's canonical transformation for each wave vector. In another case, inspired by Nozières and Saint James the canonical transformation for 0 wave vector is replaced by a shift in the creation/annihilation operators. The following were proved: For the VB basis the lowest energy is obtained in a state with $\propto \sqrt{volume}$ quasiparticles in the zero mode. The number of physical particles in the zero mode is of the order of the volume and its fluctuation is anomalously large, resulting in an excess energy. The same fluctuation is normal in the second type of optimized bases, the minimum energy is smaller and is attained in a vacuum state. Associated quasiparticle theories and questions about the gap in their spectrum were also discussed.

E-Mail:

Ferenc Iglói	igloi@szfki.hu
Róbert Juhász	juhasz@szfki.hu
István Kovács	ikovacs@szfki.hu
Nóra Menyhárd	menyhard@szfki.hu
András Sütő	suto@szfki.hu
Zsolt Szép	szepzs@achilles.elte.hu
Péter Szépfalusy	psz@galahad.elte.hu

Grants and international cooperations

OTKA T048721	Statistical physics of disordered systems (F. Iglói, 2005-2008)
OTKA T046129	Dynamics of phase transitions and symmetry breaking phases (P. Szépfalusy, 2004-2008)
MTA-DFG/193	Statistical physics of disordered systems (F. Iglói, 2008-2009)

Publications

Articles

B.1. Lajkó* P, Turban* L, Iglói F; Scaling properties at the interface between different critical subsystems: The Ashkin-Teller model; *Phys Rev B*; **76**, 224423/1-9, 2007

B.2. Juhász R; Anomalous transport in disordered exclusion processes with coupled particles; *J Stat Mech;* P11015/1-19, 2007

B.3. Iglói F, Juhász R; Exact relationship between the entanglement entropies of XY and quantum Ising chains; *Europhys Lett;* **81**,57003/1-6, 2008

B.4. Környei* L, Pleimling* M, Iglói F; Nonequilibrium critical dynamics of the two-dimensional Ising model quenched from a correlated initial state; *Phys Rev E;* **77**, 011127/1-6, 2008

B.5. Iglói F, Kovács* IA; Griffiths-McCoy singularities in random quantum spin chains: Exact results; *Phys Rev B*; **77**, 144203/1-7, 2008

B.6. Iglói F, Lin* Y-C; Finite-size scaling of the entanglement entropy of the quantum Ising chain with homogeneous, periodically modulated and random couplings; *J Stat Mech;* P06004/1-18, 2008

B.7. Iglói F, Turban* L; Aperiodic Ising model on the Bethe lattice: Exact results; *Phys Rev E*; **78,** 031128/1-7, 2008

B.8. Juhász R; Random walks in a random environment on a strip: a renormalization group approach; *J Phys A: Math Theory*; **41**, 315001/1-7, 2008

B.9. Sütő A, Szépfalusy P; Variational wave functions for homogenous Bose systems; *Phys Rev A;* **77**, 023606/1-14, 2008

B.10. Ódor* G, Menyhárd N; Crossovers from parity conserving to directed percolation universality; *Phys Rev E;* **78**, 041112/1-7, 2008

B.11. Kovács* P, Szép Zs; Influence of the isospin and hypercharge chemical potentials on the location of the CEP in the μ_B-T phase diagram of the $SU(3)_L XSU(3)_R$ chiral quark model; *Phys Rev D***; 77,** 065016/1-13, 2008

B.12. Fejős* G, Patkós* A, Szép Zs; Renormalisability of the 2PI-Hartree approximation of multicomponent scalar models in the broken symmetry phase; *Nucl Phys A***; 803**, 115-135, 2008

B.13. Patkós* A, Szép Zs; Counterterm resummation for 2PI-approximation in constant background; *Nucl Phys A***; 811**, 329-352, 2008

See also: E.3., E.20.

C. ELECTRONIC STATES IN SOLIDS

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

The surface core-level binding-energy shift (SCLS) of Pd at the AgcPd1-c(111) surface was calculated as a function of bulk concentration of the alloy. The equilibrium volume and the surface concentration profile used in the calculations refer to the 0 K case. The SCLSs were evaluated within the Z+1 approximation. The results were analyzed using the mixing enthalpy of the alloy and the bulk and surface chemical potentials. A relation of the SCLS to the bulk concentration was considered. This relation was shown to be mediated by the surface concentration profile which induces the observed nonlinear behavior. The results were interpreted using a simple model for the alloy electronic structure.

Using first-principles quantum-mechanical theory, we demonstrated that the surface chemistry of Fe-Cr alloys follows the peculiar threshold behavior characteristic of ferritic stainless steels. We found that in dilute alloys the surfaces are covered exclusively by Fe, whereas for bulk Cr concentration above ~10% the Cr-containing surfaces become favorable. The two distinctly dissimilar surface regimes appear as a consequence of two competing magnetic effects: the magnetically induced immiscibility in bulk Fe-Cr alloys and the stability of magnetic surfaces.

The stacking fault energies are used to illustrate the footprint of magnetism on the mechanical properties of Fe–Cr–Ni alloys forming the basis of austenitic stainless steels. We found that the usual chemical effects of alloying additions are accompanied by major magnetic effects, which stabilize the most common industrial alloy steels at normal service temperatures. We suggested that part of the uncertainties associated with the experimental data on the stacking fault energies are due to the strong concentration and temperature dependence originating from the persisting local magnetic moments.

We presented the first theoretical evidence of chemical composition driven superconductivity in acceptor-doped silicon and germanium, using density functional theory. We examined the concentration dependence of T_c in B-doped Si and Ge and predicted that B-doped Ge is a superconductor with a slightly higher T_c than B-doped Si. We showed that there is a critical concentration above which B-doped Si and Ge become superconducting and estimated it to be ~2.6% in Si:B and ~2.2% in Ge:B. Considering the Al-doped Si and Ge, we pointed out the decisive role of the chemical element in the hole-doping scenario.

First-principles phase diagrams of bismuth-stabilized GaAs and InP in the (100) surfaces demonstrated for the first time the presence of anomalous (2x1) reconstructions, which disobey the common electron counting principle. Combining these theoretical results with our scanning-tunneling-microscopy and photoemission measurements, we identified novel (2x1) surface structures, which are composed of symmetric Bi-Bi and asymmetric mixed Bi-As and Bi-P dimers, and found that they are stabilized by stress relief and pseudogap formation.

Due to the lower compressibility of the close-packed crystallographic planes compared to the less close-packed ones, the open free surfaces of the late transition and noble metals are generally expected to become thermodynamically stable with increasing pressure.

[#] PhD student

[+] Permanent position: Budapest University of Technology and Economics

Surface segregation in concentrated alloys and heteroepitaxial growth are possible mechanisms to create additional lattice strain around the surface layer and, thus, alter the surface stability at ambient conditions. We demonstrated this phenomenon in the case of PdAg random alloys by performing *ab initio* density functional calculations for the surface energy and stress. Our findings reveal anomalous surface stability, so far experienced only in some magnetic transition metals, and exceptionally large excess surface stress as an indicator for surface reconstruction.

Most of the engineering materials are alloys (solid solutions) and inevitably contain some impurities or defects such as vacancies. However, theoretical predictions of the hardness of this kind of materials have rarely been addressed in literature. A hardness formula for multicomponent covalent solid solution was proposed by us based on the work of Šimůnek and Vackár. With this formula, the composition dependence of the hardness was investigated for titanium nitrogencarbide ($TiN_{1-x}C_x$), off-stoichiometric transition-metal nitrides (TiN_{1-x} and VN_{1-x}), and B-doped semiconductors. The predicted hardness is in good agreement with experiments. To investigate the most frequently quoted correlation between hardness and elastic modulus, the elastic moduli of the systems involved have also been calculated. The results show that the elastic moduli cannot be used for rigorous predictions of the hardness of the solid solutions.

By considering GaAs(110) and Si(100)(2x1) surfaces, it was shown that the use of the pseudohydrogen atoms to saturate the dangling bonds at one side of the slab modeling a free surface can lead to distorted surface core-level shifts within the complete screening picture. The effect is linked to the polarization of the slab and to the change in the bulk-like electronic structure close to pseudohydrogenated part of the slab. It was demonstrated that these problems can be avoided if the pseudohydrogenated slab is large enough and the bulk reference layer is properly chosen. One easy way to control these errors is to monitor the planar-averaged potential energy curve of the slab.

First-principles total energy calculations indicate anomalously large surface relaxations for group IVA and VIIA hcp metals. In addition, for group VIIA elements the magnitude of the layer relaxation exhibits an unusually slow decay with the distance from the surface. We argued that the above phenomena can be traced back to the peculiar Fermi surface of group IVA and VIIA hcp metals. Namely, the anomalous surface relaxation appears as a consequence of low energy excitations with near $2k_F$ wave vectors, which is also reflected by the flat and degenerate d-bands located close to the Fermi level in the L-A-H plane of the hcp Brillouin-zone.

Using density functional theory formulated within the framework of the exact muffin-tin orbitals method, we investigated the elastic properties of hexagonal closed-packed Fe-Mg alloys, containing 5 and 10 atomic % Mg, up to pressures of the Earth's inner core. We demonstrated the effect of Mg alloying on the hexagonal axial ratio, elastic constants, density and sound wave velocities. We found that 10% Mg alloying decreases the shear modulus of iron by 23% and reduces the transverse sound velocity by 12% at core pressures. Our results support Mg as a candidate light element in the core.

We studied the RKKY interaction between magnetic impurities on the vicinal surfaces of transition metals through a large series of first principles calculations. We found markedly different behaviour on each of the surfaces. Namely on the (100) surface we found RKKY oscillations on neither of the hosts (AuAg, Cu), the interactions decay exponentially. On the (111) surface – in agreement with the literature – the interactions are mediated by the well known Shockley surface state. We also investigated the consequences of the Rashba splitting of the surface state, and found that on the gold surface the strong spin-orbit

interaction causes a rather large splitting and this splitting results the splitting of the oscillation frequencies accordingly.

The ab-initio electronic structure calculations were combined with a Monte Carlo method in order to study the magnetic properties of surface Co nanostructures on a Au(111) surface. We performed an ab-initio study of the ordered phases of IrMn and $IrMn_3$, the most widely used industrial anti-ferromagnets. We found extremely strong second order anisotropy for $IrMn_3$ appearing in its frustrated triangular magnetic ground state, a surprising fact since the ordered phase has a cubic symmetry. To explore the limitations of the mean-field approximation for the out-of-equilibrium Anderson model, frequently used in ab-initio molecular electronics calculations, we studied an out-of-equilibrium Anderson impurity model in a scattering formalism. We found that the mean-field approximation thus fails in every region where it predicts local moment formation.

E-Mail:

Krisztina Kádas	kadas@szfki.hu
János Kollár	jk@szfki.hu
Bence Lazarovits	bl@szfki.hu
Eszter Simon	esimon@szfki.hu
István Tüttő	tutto@szfki.hu
Balázs Újfalussy	bu@szfki.hu
Attila Virosztek	viro@szfki.hu
Levente Vitos	lv@szfki.hu
Viktor Zólyomi	zachary@szfki.hu

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. Ropo* M, Kokko* K, Punkkinen* MPJ, Hogmark* S, Kollár J., Johansson* B, Vitos L;Theoretical evidence of the compositional threshold behavior of FeCr surfaces; *Phys Rev B Rapid Communications*; **76**, 220401(R)/1-4, 2007

C.2. Kádas K, Vitos L, Ahuja* R, Johansson* B, Kollár J; Temperature dependent elastic properties of α-beryllium from first principles theory; *Phys Rev B;* **76**, 235109/1-6, 2007

C.3. Music* D, Takahashi* T, Vitos L, Asker* C, Abrikosov* IA, Schneider* JM; Elastic properties of Fe-Mn random alloys studied by *ab initio* calculations; *Applied Physics Letters*; **91**, 191904/1-3, 2007

C.4. Ványolos* A, Dóra* B, Virosztek A; Unconventional charge density wave arising from electron-phonon interaction**;** *J Supercond and Novel Magn*; **20**, 643-645, 2007

C.5. Maki* K, Dóra* B, Ványolos* A, Virosztek A; d-wave density waves in high T_c cuprates and $CoIn_5$; *Physica C*; **460-462**, 226-229, 2007

C.6. Laukkanen* P, Punkkinen* MPJ, Komsa* HP, Ahola-Tuomi* M, Kokko* K, Kuzmin* M, Adell* J, Sadowski* J, Perälä* RE, Ropo* M, Rantala* TT, Väyrynen* IJ, Pessa* M, Vitos L, Kollár J, Mirbt* S, Johansson* B; Anomalous bismuth-stabilized (2x1) reconstructions on GaAs(100) and InP(100) surfaces; *Phys Rev Lett*; **100**, 086101/1-4, 2008

C.7. Vitos L, Ropo* M, Kokko* K, Punkkinen* MPJ, Kollár J, Johansson* B; Exceptional surface stability in late transition metal alloys driven by lattice strain; *Phys Rev B Rapid Communications;* **77,** 121401(R)/1-4, 2008

C.8. Punkkinen* MPJ, Laukkanen* P, Komsa* HP, Ahola-Tuomi* M, Räsänen* N, Kokko* K, Kuzmin* M, Adell* J, Sadowski* J, Perälä* RE, Ropo* M, Rantala* TT, Väyrynen* IJ, Pessa* M, Vitos L, Kollár J, Mirbt* S, Johansson* B; Bismuth-stabilized (2x1) and (2x4) reconstructions on GaAs(100) surfaces: A combined first-principles, photoemission and scanning tunneling microscopy study; *Phys Rev B*; **78**, 195304/1-10, 2008

C.9. Vitos L, Korzhavyi* PA, Nilsson* JO, Johansson* B; Stacking fault energy and magnetism in austenitic stainless steels; *Physica Scripta*; **77**, 065703/1-3, 2008

C.10. Kádas K, Vitos L, Ahuja* R; Theoretical evidence of a superconducting transition in doped silicon and germanium driven by a variation of chemical composition; *Applied Physics Letters;* **92**, 052505/1-3, 2008

C.11. Koci* L, Ahuja* R, Vitos L, Pinsook* U; Melting of Na at high pressure from ab initio calculations; *Phys Rev B;* **77**, 132101/1-4, 2008

C.12. Kádas K, Vitos L, Ahuja* R; Elastic properties of iron-rich hcp Fe-Mg alloys up to Earth's core pressure; *Earth and Planetary Science Letters;* **271**, 221-225, 2008

C.13. Hu* QM, Kádas K, Hogmark* S, Yang* R, Johansson* B, Vitos L; Hardness and elastic properties of covalent/ionic solid solutions from first-principles theory; *J Appl Phys;* **103**, 083505/1-9, 2008

C.14. Q. M. Hu* , K. Kádas, S. Hogmark* , R. Yang* , B. Johansson* , L. Vitos; Erratum: Hardness and elastic properties of covalent/ionic solid solutions from first-principles theory; *J App Phys;* **104**, 039901/1-1, 2008

C.15. Ropo* K, Kokko* K, Vitos L; Assessing the Perdew-Burke-Ernzerhof exchange-correlation density functional revised for metallic bulk and surface systems; *Phys Rev B;* **77**, 195445/1-6, 2008

C.16. Punkkinen* MPJ, Kokko* K, Vitos L, Laukkanen* P, Airiskallio* E, Ropo* M, Ahola-Tuomi* M, Kuzmin* M, Väyrynen* IJ, B. Johansson* B; Calculation of surface core-level shifts within complete screening: Problems with pseudohydrogenated slabs; *Phys Rev B*; **77**, 245302/1-7, 2008

C.17. Hu* QM, Li* SJ, Hao* YL, Johansson* B, Yang* R, Vitos L; Phase stability and elastic moduli of Ti alloys containing Nb, Zr, and/or Sn from first-principles calculations; *Appl Phys Lett;* **93**, 121902/1-3, 2008

C.18. Shiozawa* H, Pichler* T, Kramberger* C, Grüneis* A, Knupfer* M, Buchner* B, Zólyomi V, Koltai* J, Kürti* J, Batchelor* D, Kataura* H; Fine tuning the charge transfer in carbon nanotubes via the interconversion of encapsulated molecules; *Phys Rev B;* **77**, 153402/1-4, 2008

C.19. Zólyomi V, Koltai* J, Rusznyák* Á, Kürti* J, Gali* Á, Simon* F, Kuzmany* H, Szabados* Á, Surján* PR; Intershell interaction in double walled and multiwalled carbon nanotubes: charge transfer and orbital mixing; *Phys Rev B;* **77**, 245403/1-8, 2008

C.20. Kavan* L, Frank* O, Green* AA, Hersam* MC, Koltai* J, Zólyomi V, Kürti* J, Dunsch* L; In situ Raman spectroelectrochemistry of single-walled carbon nanotubes: Investigation of materials enriched with (6,5) tubes; *J Phys Chem C;* **112**, 14179-14187, 2008

C.21. Zólyomi V, Koltai* J, Kürti* J, Pekker S; Theoretical study of the electronic structure of fullerene-cubane cocrystals; *Phys Rev B;* **78**, 115405/1-6, 2008

C.22. Dóra* B, Gulácsi* M, Koltai* J, Zólyomi V, Kürti* J, Simon* F; Electron spin resonance signal of Luttinger liquids and single-wall carbon nanotubes; *Phys Rev Lett*; **101**, 106408/1-4, 2008

C.23. Simon* F, Galambos* M, Quintavalle* D, Náfrádi* B, Forró* L, Koltai* J, Zólyomi V, Kürti* J, Nemes* NM, Rümmeli* MH, Kuzmany* H, Pichler* T; Electron spin resonance in alkali doped SWCNTs; *phys stat sol (b);* **245**, 1975-1978, 2008

C.24. Zólyomi V, Koltai* J, Kürti* J, Pekker S; The electronic band structure of fullerene-cubane cocrystals; *phys stat sol (b);* **245**, 2018-2021, 2008

C.25. Koltai* J, Zólyomi, J. Kürti* J; Phonon dispersion of small diameter semiconducting chiral carbon nanotubes – a theoretical study*; phys stat sol (b);* **245**, 2137-2140, 2008

C.26. Kürti* J, Koltai* J, Zólyomi V; Theoretical study of the electronic structure and the totally symmetric vibrations of selected CoMoCat carbon nanotubes; *phys stat sol (b);* **245**, 2141-2144, 2008

C.27. Horváth* B, Lazarovits B, Sauret* O, and Zaránd* G; Failure of the mean-field approach in the out-of-equilibrium Anderson model; *Phys Rev B;* **77**, 113108/1-4, 2008

C.28. Zólyomi V, Kollár J, Vitos L; Anomalous surface relaxation in hcp transition metals; *Phys Rev B*; **78**, 195414/1-5, 2008

C.29. Zólyomi V, Kollár J, Vitos L; On the surface relaxation of hcp transition metals; *Phil Mag B;* **88**, 2709-2714, 2008

C.30. Szunyogh* L, Lazarovits B, Udvardi* L, Jackson* J, Nowak* U; Giant magnetic anisotropy of the bulk anti-ferromagnets IrMn and IrMn3; *Cond Mat [other]*; *arXiv*:0808.3900, accepted for publication

C.31. Mattesini* M, Buforn* E, Udias* A, Vitos L, Ahuja* R; An *ab initio* study of S-substituted iron-nickel-silicon alloy at the Earth's inner core pressure; *High Pressure Research;* accepted for publication

C.32. Antal* A, Lazarovits B, Udvardi* L, Szunyogh* L, Ujfalussy B, Weinberger* P; First principles calculations of spin interactions and the magnetic ground states of Cr trimers on Au(111); *Phil Mag B*; accepted for publication

C.33. Simon E, Lazarovits B, Szunyogh* L, Ujfalussy B; Ab-initio investigation of RKKY interactions on metetallic surfaces; *Phil Mag B;* accepted for publication

C.34. Anta* A, Lazarovits B, Balogh* L, Udvardi* L, and Szunyogh* L ; Multiscale studies of complex magnetism of nanostructures based on first principles; *Phil Mag B;* accepted for publication

Conference proceeding

C.35. Ropo* M, Kokko* K, Punkkinen* MPJ, Hogmark* S, Kollár J, Johansson* B, Vitos L; Threshold behavior of FeCr alloys surface; In: 6th *European Stainless Steel Conference*; Ed.: P. Karjalainen and S. Hertzman, ISBN 91-974131-9-4, Helsinki, Finland; pp. 323-326, 2008

Book chapter

C.36. Zólyomi V, Koltai* J, Kürti* J and Kuzmany* H; Phonons of single walled carbon nanotubes"; In: *DFT Calculations on Fullerenes and Carbon Nanotubes*; eds. V. A. Basiuk and S. Irle, Research Signpost, 2008, accepted for publication

D. NON-EQUILIBRIUM ALLOYS

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

Sequence permutated multilayers. — Mössbauer spectroscopy is widely used to study nano-scale multilayers. The ^{57}Fe marker method, when the position of a thin ^{57}Fe layer is varied across the natural Fe layer, detected differences of bottom and top interface of the Fe layer in several multilayer structures. The application of the above method is limited by possible mixing and diffusion between the ^{57}Fe and the natural Fe layers. We presented a new approach which works also for cases where diffusion and mixing of the subsequent layers takes place during either sample deposition or post-annealing. In order to distinguish the bottom and top interface of the Fe layer a third element is interleaved, and the multilayers composed of three different elemental layers are deposited by sequence permutation in two different forms. The Fe/B multilayer system is chosen to be studied this way because a significant mixing of the elements occurs at the interfaces already during the sample deposition and Ag will be interleaved, since it does not mix with either of the two elements. In samples with different permutation of the layer sequence each element pair has different type of interfaces, e.g. B on top or at the bottom of the Fe layer.

Mössbauer spectra of samples measured at room temperature are shown in Fig. 1 and the evaluated hyperfine field distributions can be found in the insets. The spectra evidently depend strongly both on the thickness of the Fe and the B layers and on the layer sequence. The dependence on the thickness of the Fe and the B layers is in qualitative agreement with the trends observed earlier for Fe-B multilayers. For Fe layer thickness smaller than the range of interface mixing only spectra of amorphous Fe-B can be observed and the HF distributions strongly depend on the ratio of the Fe and the B layer thickness. When the Fe layer thickness is larger than the range of interface mixing a sub-spectrum characteristic to pure bcc-Fe layer can be identified as a sharp peak of the HF distribution close to 33 T. This was found to occure above 2 nm Fe layer thickness in case of Fe-B multilayers, where both bottom and top interfaces of Fe were formed by B intermixing. In the present case bcc-Fe like layer appears roughly above 1 nm for both layer sequences, as it can be deduced both from the ratio of the sharp sextets in the spectra of samples A1 and B1 and from the lack of sharp sextets in case of samples A2 and B2. The intermixed region of the Fe layer is reduced as compared to Fe-B multilayers since the Fe-Ag interfaces are much sharper than the Fe-B interfaces.

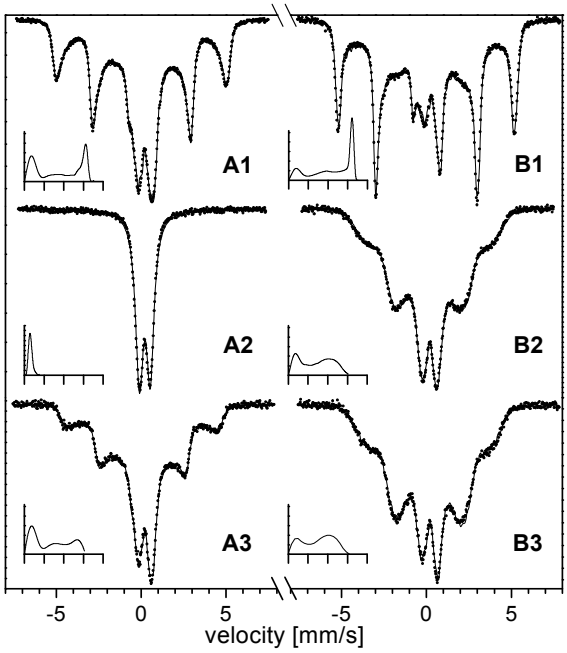


Figure 1: Room temperature Mössbauer spectra of multilayer sample pairs with Ag/Fe/B (A1, A2, A3) and Ag/B/Fe (B1, B2, B3) layer sequence. The as-prepared samples had the following layer structures: Si / [5 nm Ag / x nm 57Fe / y nm B]4 / 50nm Ag / 100nm B and Si / [5 nm Ag / y nm B / x nm 57Fe]4 / 50nm Ag / 100nm B in case of A and B samples, respectively, with x=2 and y=2 for A1 and B1, x=1 and y=1 for A2 and B2, and x=1 and y=0.33 for A3 and B3. The evaluated hyperfine field distributions are shown in insets in the 0 to 40 T range.

Measurements of these samples at low temperatures and in high magnetic fields undoubtedly show that the B concentration distribution of the Fe-B interface is different in the sequence permutated sample pairs. Intermixing is larger at the interface where B is on top of the Fe layer. Transmission electron microscopy measurements showed a much larger interface roughness for the Fe/B/Ag than for the B/Fe/Ag sequence multilayers. It is due to the different growth process of Ag on B and Fe and it can influence the Fe-B interface properties, as well. The difference of top and bottom interface of Fe with B was also found in trilayer samples, where Ag is grown over B only as a cover layer. This shows that the role of the layers sequence dependent growth of the 5 nm thick interleaved Ag layer is small in the Fe-B interface formation and the difference of top and bottom interfaces of Fe with B should be explained by a different diffusion mechanism for the two cases.

Investigation of nanocrystalline alloys. — Temperature dependence, from room temperature up to 1000 K, of the initial permeability (μ) of $Fe_{83-x}Co_xGe_5Zr_6B_5Cu_1$ (x=5 and 20) alloys at different stages of devitrification is reported. As nanocrystallization progresses, the room temperature μ decreases but the high temperature one increases, leading to an improvement of the thermal stability of μ in the 300 K – 915 K temperature range. It is characterized by a temperature coefficient of permeability ~0.1%/K ($\mu \sim 4000$) and 0.04%/K ($\mu \sim 800$) for 5 and 20 at. % Co containing alloys, respectively.

Investigation of the magnetocaloric effect. — The magnetic entropy change has been studied in $Fe_{92-x}Cr_8B_x$ (x=12, 15) amorphous alloys. Increasing the B content, the peak entropy changes and the Curie temperature of the alloy increases. This is in agreement with an increase in the average magnetic moment per iron atom. The thermal and field dependences of the magnetic entropy change curves have been analyzed with the use of the Arrott–Noakes equation of state. It is shown that determining the parameters in this equation of state (through fitting the magnetization data) allows prediction of the field and temperature dependences of the magnetic entropy change curves in a broad temperature range around the Curie temperature.

E-Mail:

Imre Vincze	vincze@szfki.hu
Sára Judit Balogh	baloghj@szfki.hu
László Bujdosó	bujdi@szfki.hu
Dénes Kaptás	kaptas@szfki.hu
Tamás Kemény	kemeny@szfki.hu
László Ferenc Kiss	kissl@szfki.hu

Grants and international cooperations

OTKA T 048965	Magnetic properties of multilayer structures (J. Balogh, 2005-2008)
OTKA K68612	Magnetic anisotropy of structures with reduced dimension (L.F. Kiss, 2007-2010)
Hungarian-Spanish	Academic Exchange Programme (Study of magnetocaloric effect in amorphous alloys and nanostructures, L.F. Kiss, 2007-2008)

Long term visitors

— Rafael Caballero Flores, University of Sevilla, Spain, from 22 September to 16 November, 2008 (T. Kemény and L.F. Kiss)

Publications

Articles

D.1. Németh* P, Böhönyey* A, Tichy* G, Kiss LF; Anomalous Curie-point relaxation in a Cr-containing amorphous alloy; *J Magn Magn Mater*; **320**, 719-723, 2008

D.2. Poulopoulos* P, Baskoutas* S, Kiss LF, Bujdosó L, Kemény T, Wilhelm* F, Rogalev* A, Kapaklis* V, Politis* C, Angelakeris* M, Saksl* K; Magnetic moments of Fe and Y in the FeBY glass forming system; *J Non-Cryst Solids*; **354**, 587-591, 2008

D.3. Kiss LF, Kemény T, Bujdosó L, Bakonyi I, Baskoutas* S, Poulopoulos* P, Kapaklis* V, Politis* C; Heterogeneous magnetism in Fe-doped bulk-amorphous and nanostructured Pd-based alloys; *J Phys: Condens Matter*; **20**, 015211/1-8, 2008

D.4. Blázquez* JS, Conde* CF, Franco* V, Conde* A, Kiss LF; Magnetic permeability of $(FeCoGe)_{88}Zr_6B_5Cu_1$ alloys: Thermal stability in a wide temperature range; *J Appl Phys*; **103**, 07E721/1-3, 2008

D.5. Kiss LF, Balogh J, Kaptás D, Kemény T, Vincze I; Magnetic properties of ball-milled Fe-rich $Fe_{50+x}Al_{50-x}$ alloys; *Rev Adv Mater Sci*; **18**, 505-508, 2008

D.6. Balogh J, Fetzer* Cs, Kaptás D, Kiss LF, Szűcs* IS, Dézsi* I, Vincze I; Perpendicular anisotropy in Fe/Ag multilayers; p*hys stat sol (a)*; **205**, 1828-1830, 2008

D.7. Franco* V, Conde* A, Kiss LF; Magnetocaloric response of FeCrB amorphous alloys: Predicting the magnetic entropy change from the Arrott-Noakes equation of state; *J Appl Phys*; **104**, 033903/1-5, 2008

D.8. Kiss LF, Kaptás D, Balogh J, Tanczikó* F, Major* M, Vincze I; Magnetic properties of Fe-Ag granular alloys; *J Alloys and Compounds*; accepted for publication

D.9. Caballero* R, Franco* V, Conde* A, Kiss LF; Influence of the demagnetizing field on the determination of the magnetocaloric effect from magnetization curves; *J Appl Phys*; accepted for publication

See also H.2.

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. Tóth[#], G. Tegze, M. Tegze

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 determined the thermodynamic properties of the orientational phase transitions of C_{60}-cubane and C_{70}-cubane cocrystals by complex calorimetric studies. We have prepared C_{60}-bis-isocyanato-cubane, a new member of the rotor-stator family with lower symmetry. We started various calculations on the stability and the dynamics of the new phases. Further, we have determined the pressure dependence of the optical spectra of cubane-fullerene cocrystals and found two phase transitions.

We extended our earlier studies on the alkali-C_{60} compounds. We have determined the electronic structure of two fullleride polymers (with lithium and magnesium) by combining our results with several other methods.

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 compared the wide-range optical spectra of several transparent nanotube films and found correlation between the average diameter, the spectral properties and the metallic nanotube content of these samples. We also determined that chemical functionalization of nanotubes by nucleophilic reagents is selective to tube diameter, preferring small diameter tubes.

[#] Ph.D. student

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 promise applications in a wide area.

We participated in a combined study of graphene and few-layer graphene crystals by AFM and Raman spectroscopy and found that this combined approach is very useful in determining the thickness of the layers.

Theory of phase transformations. — Advanced phase-field techniques we developed earlier have been applied to address various aspects of polycrystalline solidification including different modes of crystal nucleation. Along this line (i) we have performed a quantitative comparison of various models of homogeneous crystal nucleation with atomistic simulations for the single-component hard sphere fluid; (ii) extending previous work for pure systems, heterogeneous nucleation in unary and binary systems is described via introducing boundary conditions that realize the desired contact angle; (iii) a quaternion representation of crystallographic orientation of the individual particles we developed has been applied for modeling a broad variety of polycrystalline structures including crystal sheaves, spherulites and those built of crystals with dendritic, cubic, rhombo-dodecahedral and truncated octahedral growth morphologies; (iv) we have also presented illustrative results for dendritic polycrystalline solidification obtained using a simple density functional theory (Fig. 1).

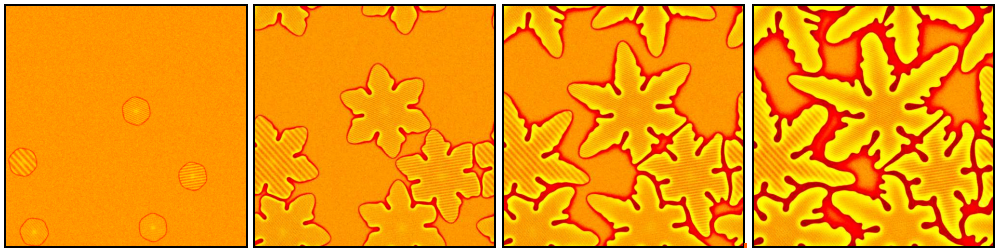


Fig. 1. *Multi-particle dendritic solidification in the binary density functional theory (the distribution of the difference of the number density fields is shown). The simulations have been performed on a 16 384 × 16 384 grid, using a semi-implicit spectral method. Note that the position of all atoms of the crystalline phase are known accurately.*

We have developed an efficient method to solve numerically the equations of dissipative dynamics of the binary density functional model proposed by Elder *et al.* characterized by variable coefficients. Using the operator splitting method, the problem has been decomposed into sub-problems that can be solved more efficiently. A combination of non-trivial splitting with spectral semi-implicit solution leads to sets of algebraic equations of diagonal matrix form. Extensive testing of the method has been carried out to find the optimum balance among errors associated with time integration, spatial discretization, and splitting. We have shown that our method speeds up the computations by orders of magnitude relative to the conventional explicit finite difference scheme, while the costs of the point-wise implicit solution per time step remains low. Also we show that due to its numerical dissipation, finite differencing cannot compete with spectral differencing in terms of accuracy. In addition, we have demonstrated that our method can efficiently be parallelized for distributed memory systems, where an excellent scalability with the number of CPUs is observed.

Ab initio structure solution. — In recent years we have developed an *ab initio* method of crystal structure determination – named charge flipping. This year we were invited to write a feature article on the method for the special issue of *Acta Cryst. A* celebrating the 60*th* birthday of the International Union of Crystallography (IUCr). In addition to reviewing the

current status and practical applications of the method, we could also include some new improvements on the basic charge flipping algorithm. These are: a better choice of the threshold parameter δ, a cleanup procedure to improve the quality of the final solution, several improvements of the dual-space iteration scheme, a new way of using normalized structure factors and various strategies of using known structural information in the iteration process. The main results of this study were presented in 2008 as two plenary lectures at the XXI Congress of the IUCr in Osaka and at the European Powder Diffraction Conference (EPDIC-11) in Warsaw, as well as tutorials at the IUCr Computing School in Kyoto.

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 damaged by the measuring process itself. Even the most often used x-rays destroy the sample during the collection of a diffraction pattern. 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 shown that a thin water tamper layer around the sample significantly slows down the deterioration of the sample. We also studied the first step of the data evaluation process, the classification. We determined the minimum sample size at various incident beam intensities, which allows successful classification.

E-Mail:

Gábor Bortel	gb@szfki.hu
Ferenc Borondics	bf@szfki.hu
Bea Botka	bbea@szfki.hu
Gyula Faigel	gf@szfki.hu
László Gránásy	grana@szfki.hu
Zoltán Jurek	jurek@szfki.hu
Katalin Kamarás	kamaras@szfki.hu
Gyöngyi Klupp	klupp@szfki.hu
Éva Kováts	kovatse@szfki.hu
László Környei	leslie@kornyei.hu
Katalin Németh	nemethk@szfki.hu
Gábor Oszlányi	go@szfki.hu
Áron Pekker	pekkera@szfki.hu
Sándor Pekker	pekker@szfki.hu
Tamás Pusztai	pusztai@szfki.hu
Zsolt Szekrényes	szezsolt@szfki.hu
György Tegze	turpi@szfki.hu
Miklós Tegze	mt@szfki.hu
Gyula Tóth	gytoth@szfki.hu

Grants and international cooperations

OTKA T 049338 Optical spectroscopy of molecular carbon structures (principal investigator: K. Kamarás, 2005-2008)

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

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

OTKA T 046700 Topochemical reactions in crystalline fullerenes and related materials (S. Pekker, 2004-2008)

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, 2005-2008)

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)

ESA PECS 98059 Phase field modeling of nucleation in fcc-bcc-liquid systems (T. Pusztai, 2007–2008)

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

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, 2006-2008)

Hungarian Academy of Sciences - Spanish Council for Advanced Research Bilateral Cooperation, 2007/2008:07, Investigation of pristine and intercalated carbon nanostructures (S. Pekker, 2007-2008)

ESP-18/2006 Hungarian - Spanish Intergovernmental S&T Cooperation, Investigation of pristine and intercalated carbon nanostructures (S. Pekker, 2007-2008)

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)

Publications

Articles

E.1. Löser* W, Hermann* R, Woodcock* TG, Fransaer* J, Krivilyov* M, Gránásy L, Pusztai T, Tóth GI, Herlach* DM, Holland-Moritz* D, Kolbe* M, Volkmann* T; Nucleation and phase selection in undercooled melts: Magnetic alloys of industrial relevance (MAGNEPHAS); *J Jpn Soc Microgravity Appl;* **25**, 319-324, 2008

E.2. Pusztai T, Tegze G, Tóth GI, Környei L, Bansel* G, Fan* Z, Gránásy L; Phase-field approach to polycrystalline solidification including heterogeneous and homogeneous nucleation; *J Phys: Condens Matter;* **20**, 404205-1-16, 2008

E.3 Oszlányi G, Sütő A; The charge flipping algorithm; *Acta Cryst A;* **64**, 123-134, 2008

E.4. Verberck* B, Heresanu* V, Rouzière* S, Cambedouzou* J, Launois* P, Kováts É, Pekker S, Vliegenthart* GA, Michel* KH, Gompper* G; Fullerene-cubane: X-ray scattering experiments and Monte Carlo simulations; *Fullerenes, Nanotubes and Carbon Nanostructures*; **16**, 293-300, 2008

E.5. Alatas* A, Said* AH, Sinn* H, Bortel G, Hu* MY, Zhao* J, Burns* CA, Burkel* E, Alp* EE; Atomic form-factor measurements in the low-momentum transfer region for Li, Be, and Al by inelastic x-ray scattering; *Phys Rev B;* **77**, 064301/1-7, 2008

E.6. Jurek Z, Faigel G; The effect of tamper layer on the explosion dynamics of atom clusters; *Eur Phys J D;* **50**, 35–43, 2008

E.7. Macovez* R, Savage* R, Venema* L, Schiessling* J, Kamarás K, Rudolf* P: Low bandgap and ionic bonding with charge transfer threshold in thin-film polymeric Li_4C_{60}; *J Phys Chem C;* **112,** 2988-2996, 2008

E.8. Quintavalle* D, Borondics F, Klupp G, Baserga* A, Simon* F, Jánossy* A, Kamarás K, Pekker S; Structure and properties of the stable two-dimensional conducting polymer Mg_5C_{60}; *Phys Rev B;* **77,** 155431/1-5, 2008

E.9. Pap* AE, Dücső* Cs, Kamarás K, Battistig* G, Bársony* I; Heavy water in gate stack processing; *Mat Sci Forum*; **573-574,** 119-131, 2008

E.10. Nemes-Incze* P, Osváth* Z , Kamarás K, Biró* LP; Anomalies in thickness measurements of graphene and few layer graphite crystals by tapping mode atomic force microscopy; *Carbon;* **46**, 1435-1442, 2008

E.11. Pekker Á, Wunderlich* D, Kamarás K, Hirsch* A; Diameter selectivity of nanotube sidewall functionalization probed by optical spectroscopy; *Phys Stat Sol (b);* **245,** 1954-1956, 2008

E.12. Kamarás K, Pekker Á, Bruckner* M, Borondics F, Rinzler* AG, Tanner* DB, Itkis* ME, Haddon* RC, Tan* Y, Resasco* DE ; Wide-range optical spectra of carbon nanotubes; a comparative study; *Phys Stat Sol (b);* **245,** 2229-2232, 2008

E.13. Thirunavukkuarasu* K, Kuntscher* CA, Borondics F, Klupp G, Kamarás K ; Infrared spectroscopy on the fullerene C_{70} under pressure; *Phys Stat Sol (b);* **245,** 2006-2009, 2008

E.14. Kuntscher* CA, Thirunavukkuarasu* K, Kamarás K, Simon* F, Walters* DA; Infrared microreflectance study of magnetically aligned single-walled carbon nanotubes under pressure; *Phys Stat Sol (b);* **245,** 2288-2291, 2008

E.15. Thirunavukkuarasu* K, Kuntscher* CA, Nagy* BJ, Jalsovszky* I, Klupp G, Kamarás K, Kováts É, Pekker S ; Orientational ordering and intermolecular interactions in the rotor-stator compounds $C_{60}{\cdot}C_8H_8$ and $C_{70}{\cdot}C_8H_8$ under pressure; *J Phys Chem C*; **112,** 17525-17532, 2008

E.16. Tegze G, Bansel* G, Tóth GI, Pusztai T, Fan* Z, Gránásy L; Advanced operator-splitting-based semi-implicit spectral method to solve the binary phase-field crystal equation with variable coefficients; *J Comput Phys*, accepted for publication

Articles in Hungarian

E.17. Faigel G, Jurek Z; Egyedi molekulák, atomfürtök atomi szerkezetének leképezése (Structural imaging of single molecules and atom clusters, in Hungarian); *Fizikai Szemle*; accepted for publication

E.18. Faigel G, Jurek Z, Bortel G; Egyedi molekulák atomi szerkezetének meghatározása (Atomic level structure determination of single molecules, in Hungarian); *Magyar Kémiai Folyóirat*; accepted for publication

Conference proceedings

E.19. Iwasiewicz-Wabnig* A, Kováts É, Pekker S, Sundqvist* B; Low-temperature optical studies of C_{60}-cubane rotor-stator compound; *J Phys: Conf Ser;* **100**, 052091, 2008

E.20. Oszlányi G, Sütő A; Introduction to the charge flipping method; *Newsletter of the Commission on Crystallographic Computing;* **9**, 83-91, 2008; (tutorial at the IUCr Computing School, Kansai Seminar House, Kyoto, 18-23 August 2008)

Book chapter

E.21. Kamarás K, Pekker Á; Identification and separation of metallic and semiconducting carbon nanotubes; In: *Handbook of Nanoscience and Technology*, Ed: Narlikar AV, Fu YY, Oxford University Press, accepted for publication

See also: C.21., C.24., G.2.

F. COMPLEX FLUIDS

Á. Buka, T. Börzsönyi, N. Éber, K. Fodor-Csorba, I. Jánossy, T. Tóth-Katona, A. Vajda

Synthesis. — New asymmetrical banana–shaped liquid crystals have been prepared. These materials have five aromatic rings connected by ester functional groups as based on our former results that helps to obtain a low melting point. The double bond bearing tail on their one end makes the molecules appropriate for further polymerization. The synthesis has been carried out in several steps using benzyl protection and acid chloride activation. These compounds are precursors of liquid crystalline elastomers. According to the electro-optical investigations the compounds exhibit ferroelectric and antiferroelectric behaviour. The mesophases appear at relatively low temperatures, e.g. in the range 110-148 ^{o}C.

Some previously synthesized bent core compounds have been mixed with calamitic materials. These mixtures have been investigated by solid state ^{2}H NMR. The pure banana compound exhibits B_2 phase, which has also been found in the mixtures. The nematic phase of the mixture may be a candidate for a biaxial phase.

Electric field driven pattern formation. — The role of flexoelectricity in electric field induced pattern formation of nematic liquid crystals has been reconsidered. The standard hydrodynamic model (SM) of electroconvection (EC) has been extended by incorporating flexoelectric effects into the governing equations. It has been shown that this extended SM provides finite instability thresholds also for materials in which the anisotropy of the dielectric permittivity and of the electrical conductivity are of the same sign, while the classical SM (without flexoelectricity) allows pattern formation at opposite signs of the anisotropies only. Thus flexoelectricity can explain the occurrence of the nonstandard EC patterns which have been detected experimentally.

An unexpected frequency dependence of the threshold voltages $U_c(f)$ has been detected in electroconvection of various nematics under the condition when the time scales of the director relaxation and the period of the driving ac voltage become comparable. For standard conductive EC $U_c(f)$ bends down considerably toward low frequencies, while for standard dielectric EC as well as for nonstandard EC it bends up strongly with the decrease of the driving frequency. It has been shown by numerical simulations using the extended SM that this behaviour is also owing to flexoelectricity.

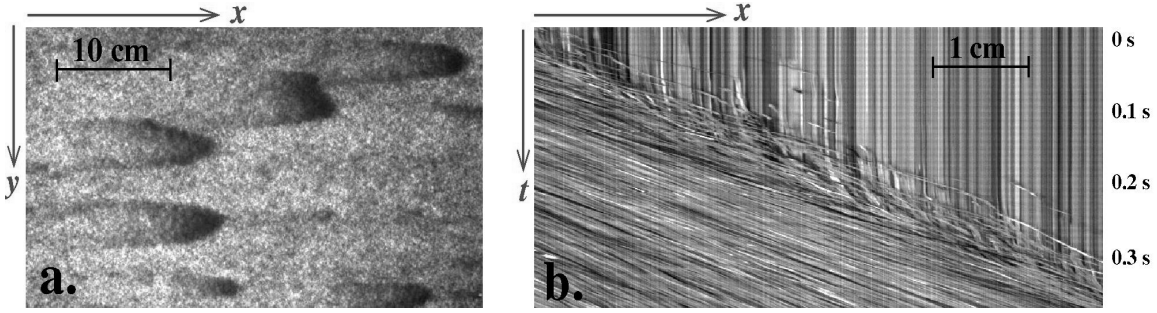
Interactions at liquid crystal surfaces. — We have explained the experimentally observed fact that radial liquid crystal droplets do not spin in circularly polarized light by taking into account both the optical torque and the radiation force acting on the droplet.

We have studied the zenithal anchoring of nematic liquid crystals using precise birefringence measurements. Director gliding at the surface has been found above a threshold reorienting electric field. The zenithal gliding had similar time characteristics to that found earlier in the case of azimuthal gliding.

Ferronematics. — Ferronematic materials have been prepared by mixing liquid crystals with magnetic nanoparticles of various shapes. Electric and/or magnetic field induced structural transitions (reorientation of the nematic director) have been detected and monitored by dielectric measurements. The addition of nanoparticles has resulted in a reduction of the critical magnetic field of the liquid crystal due to the increase of the net magnetic susceptibility anisotropy; the effect was more pronounced for nanoparticles of elongated shape. Doping the system with nonvolatile solvents a wide two-phase region featuring ferronematic droplets has been established at the isotropic-nematic phase transition. The droplets undergo similar structural transitions under the influence of

external fields. The above measurements allowed the determination of the type and strength of the anchoring of liquid crystal molecules on the nanoparticle's surfaces which was found to depend on the shape of the nanoparticles.

Granular flow. — Properties of avalanches in gravitationally forced granular layers on a rough inclined plane have been determined experimentally for different materials and for a variety of grain shapes ranging from spherical beads to highly anisotropic particles with dendritic shape. Figure (a) exhibits such avalanches in transmitted light (top view). The front velocity has been measured and correlated with the area and height for many avalanches. Increasing the shape irregularity of the grains a dramatic qualitative change has been detected in avalanche properties. For rough nonspherical grains the avalanches are faster, bigger, and overturning, i.e. the down-slope speed of individual particles exceeds the front speed, in contrast to avalanches of spherical glass beads which are slower, smaller and where particles always travel slower than the front speed. The particle dynamics at the front is illustrated for sand in Figure (b) where grain trajectories are shown in an *x-t* plot. Three quantities: (i) the dimensionless avalanche height, (ii) the ratio of particle to front speed, and (iii) the growth rate of the avalanche speed with increasing avalanche size exhibit a linear increase with $\tan\theta$ or with β, where θ is the bulk angle of repose, and β the slope of the depth averaged flow rule. Here both θ and β reflect the grain shape irregularity. These relations provide a tool for predicting important dynamical properties of avalanches as a function of grain shape irregularity. For further details and movies visit the web-site: http://www.szfki.hu/~btamas/gran/avalanche.html



E-Mail:

Tamás Börzsönyi	btamas@szfki.hu
Ágnes Buka	ab@szfki.hu
Nándor Éber	eber@szfki.hu
Katalin Fodor-Csorba	fodor@szfki.hu
István Jánossy	janossy@szfki.hu
Tibor Tóth-Katona	katona@szfki.hu
Anikó Vajda	vajda@szfki.hu

Grants and international cooperations

OTKA K 061075 Mesogens with polar ordering of non-chiral building blocks (Á. Buka, 2006-2009)

OTKA F-060157 Experimental studies of dynamical processes in granular materials (T. Börzsönyi, 2006-2008)

EU-MSCF-CT-2004-013119 Interactive training and research in nonlinear science from physics to biology (Á. Buka, 2004-2008)

COST D35 WG 13-05. Molecular switches based on liquid crystalline materials (K. Fodor-Csorba, 2005-2008)

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

KPI TÉT SK-19/2006 (Hungarian-Slovak bilateral) Ferronematic materials (N. Éber, 2007-2008)

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-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)

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

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

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

ECO-NET 2008 N° 18843TM: Surface memory and gliding of liquid crystals: physical mechanisms and connection with anchoring energy (I. Jánossy, 2008)

Long term visitors

— Shingo Tanaka: Tokyo Institute of Technology, Tokyo, Japan, 17 February – 15 March, 2008 (MTA-JSPS, host: Éber N)

— Pramod Kumar: Centre for Liquid Crystal Research, Jallahalli, Bangalore, India, 3 May – 31 July, 2008 (MTA-INSA, host: Éber N)

— Prof. Antal Jákli: Liquid Crystal Institute, Kent State University, Kent, USA, 2 June - 12 July, 2008 (host: Éber N)

— Jake Fontana: Kent State University, Kent, USA, 14 June - 15 July, 2008 (host: Jánossy I)

— Prof. David Statman: Allegheny College, Meadville, USA, 16 June – 15 July, 2008 (host: Jánossy I)

— Matthew Kerr: Allegheny College, Meadville, USA, 16 June – 15 July, 2008 (host: Jánossy I)

— Shad Hopson: Allegheny College, Meadville, USA, 16 June – 15 July, 2008 (host: Jánossy I)

— Joshua Levinson: Allegheny College, Meadville, USA, 16 June – 15 July, 2008 (host: Jánossy I)

— Lu Shi: Tokyo Institute of Technology, Tokyo, Japan, 26 August – 26 September, 2008 (MTA-JSPS, host: Fodor-Csorba K.)

Publications

Articles

F.1. Coleman* DA, Jones* CD, Nakata* M, Clark* NA, Walba* DM, Weissflog* W, Fodor- Csorba K, Watanabe* J, Novotna* V, Hamplova* V; Polarization splay as the origin of modulation in the B_1 and B_7 smectic phases of bent-core molecules; *Phys Rev E;* **77**, 021703/1-6, 2008

F.2. Nair* GG, Bailey* C, Taushanoff* S, Fodor-Csorba K, Vajda A, Varga* Z, Bota* A, Jákli* A; Electrically tunable color of mixtures of bent-core and rod-shaped molecules; *Adv Mater;* **20,** 3138-3142, 2008

F.3. Dorjgotov* E, Fodor-Csorba K, Gleeson* JT, Sprunt* S, Jákli* A; Viscosities of a bent-core nematic liquid crystal; *Liquid Crystals*; **35,** 149-155, 2008

F.4. Krekhov* A, Pesch* W, Éber N, Tóth-Katona T, Buka Á; Nonstandard electroconvection and flexoelectricity in nematic liquid crystals; *Phys Rev E;* **77**, 021705/1-11, 2008

F.5. Tóth-Katona T, Éber N, Buka Á, Krekhov* A; Flexoelectricity and competition of time scales in electroconvection; *Phys Rev E;* **78**, 036306/1-12, 2008

F.6**.** Statman* D, Basore* V, Sulai* Y, Dunlap* B, Jánossy I; Photoinduced gliding of the surface director in azo-dye doped nematic liquid crystals; *Liquid Crystals;* **35**, 33-38, 2008

F.7**.** Jánossy I; Electromagnetic torque and force in axially symmetric liquid crystal droplets; *Optics Letters;* **33**, 2371–2373, 2008

F.8. Tomašovičová* N, Kopčanský* P, Koneracká* M, Tomčo* L, Závišová* V, Timko* M, Éber N, Fodor-Csorba K, Tóth-Katona T, Vajda A, Jadzyn* J; The structural transitions in 6CHBT-based ferronematic droplets; *J Phys Condens Matter;* **20**, 204123/1-5, 2008

F.9. Tomašovičová* N, Koneracká* M, Kopčansky* P, Timko* M, Závišová* V, Vajda A, Fodor-Csorba K, Éber N, Tóth-Katona T; The anchoring energy of liquid crystal molecules to magnetic particles in HAB-based ferronematics; *Acta Physica Polonica A;* **113**, 591-594, 2008

F.10. Kopčanský* P, Tomašovičová* N, Koneracká* M, Závišová* V, Timko* M, Džarová* A, Šprincová* A, Éber N, Fodor-Csorba K, Tóth-Katona T, Vajda A, Jadzyn* J; Structural changes in the 6CHBT liquid crystal doped with spherical, rodlike, and chainlike magnetic particles; *Phys Rev E;* **78**, 011702/1-5, 2008

F.11. Börzsönyi T, Halsey* TC, Ecke RE; Avalanche dynamics on a rough inclined plane; *Phys Rev E*; **78**, 011306/1-15, 2008

F.12. May* M, Schöpf* W, Rehberg* I, Krekhov* A, Buka Á; Transition from longitudinal to transversal patterns in an anisotropic system; *Phys Rev E*; accepted for publication

Article in Hungarian

F.13. Buka Á, Éber N; Konvekció égen, földben, vízben és folyadékkristályokban (Convection in the sky, in earth, in water and in liquid crystals, in Hungarian); *Fizikai Szemle*; **58**, 359-361, 2008

Conference proceedings

F.14. Jákli* A, Chambers* M, Harden* J, Madhabi* M, Teeling* R, Kim* J, Li* Q, Nair* GG, Éber N, Fodor-Csorba K, Gleeson* JT, Sprunt* S; Extraordinary properties of nematic phases of bent-core liquid crystals; In: *Emerging Liquid Crystal Technologies III, San Jose, January 20-24, 2008*; Ed.: Chien L-C, Proc. SPIE, Vol **6911**, 691105/1-10, 2008

F.15. Fodor-Csorba K, Jákli* A, Eremin* A, Hamplova* V, Kaspar* M, Novotna* V, Kohout* M, Gomola* K, Pociecha* D, Vajda A, Veracini* CA, Galli* G; Chiral and achiral banana shaped liquid crsytals, synthesis and characterization; In: *German Topical Meeting on Liquid Crystals, Magdeburg, Germany, March 12-14, 2008*; pp. 15-18, 2008

F.16. Tóth Katona T, Éber N, Krekhov* A, Buka Á; Competing time-scales in electroconvection; In: *Proc of the 36th German Topical Meeting on Liquid Crystal Magdeburg, Germany, March 12-14, 2008;* p. 109-112, 2008

F.17. Kopcansky* P, Tomasovicova* N, Koneracka* M, Zavisova* V, Timko* M, Dzarova* A, Sprincova A* Tomco* L, Éber N, Fodor-Csorba K, Tóth Katona T, Vajda A, Jadzyn* J; The role of shape of fine magnetic particles on structural transitions in ferronematics; In: *Proc of the 7th PAMIR International Conference – Fundamental and Applied MHD and COST P17 Annual Workshop, Presquile de Giens, France, Sept 8-12, 2008;* Vol 2/2, pp. 691-695, 2008

G. ELECTRON CRYSTALS

G. Kriza, P. Matus, Gy. Mihály[+], Á. Pallinger[#], B. Sas, F.I.B. Williams

Dissipation in high-T_c superconductors. — We investigate monocrystalline $Bi_2Sr_2Ca_2CuO_8$ (BSCCO) which exemplifies well the generic properties of the family of cuprate superconductors: type II superconductivity with high, doping-tunable critical temperature and strong anisotropy describable as a stack of superconducting planes weakly coupled together by Josephson tunnelling. Our interest lies in the behaviour of the vortices created on applying a magnetic field perpendicular to the planes and how their interactions with themselves and with the host disorder affect dissipation under current flow. Figure 1 shows the generally accepted vortex (*H-T*) phase diagram for optimally doped (maximum T_c) BSCCO. The classic Abrikosov phase with vortices aligned from plane to plane only exists at low field; higher field decreases the effectiveness of the Josephson coupling in aligning the vortices and, at low temperature, a quasi 2-D glass phase of "pancake" vortices in each plane is favoured with evanescent correlation between planes. This phase is characterised by dissipationless transport at small currents with a distinct vortex depinning threshold. The upper limit of the phase is seen in the reversibility of the magnetic moment, $T_{irr}(H)$ in Fig. 1, indicating finite conductivity although the *V-I* characteristic remains nonlinear up to a limiting temperature $T_{lin}(H) < T(H_{c2})$ beyond which it seems that the vortices behave as a simple viscous liquid.

Superimposed on this simple picture is an unexplained locus $T_{ms}(H)$ below which metastability of the *V-I* response sets in. Does it represent another phase boundary or perhaps a dynamic crossover of some sort? In the hope of gaining more insight into the underlying cause, we have undertaken a series of experiments on highly underdoped BSCCO in collaboration with the Ecole Polytechnique Fédérale de Lausanne. We have discovered that the phenomena of sensitivity to field and temperature cycling are similar to the optimal doped case but that the locus of onset does not scale in the same way as the accepted phase boundary lines but scales simply with T_c. We have been able to construct a model for the dynamics of structural disorder which accounts well for all the observed behaviours to field and temperature cycling as well as for the scaling with T_c and the form of the function $T_{ms}(H)$. It is based on the interplay between the elastic energy of the lattice and the attraction of point defect vortex traps in the superconductor. The appearance of metastability is a sign of disconnection of the vortex/trap system, represented as an asymmetric double well, from the thermal bath on the time scale of the experiment duration. It is therefore not to be interpreted as a further phase transition but as a dynamic crossover. It shows too that unlike 3-D glasses, 2-D glasses are not structurally frozen at

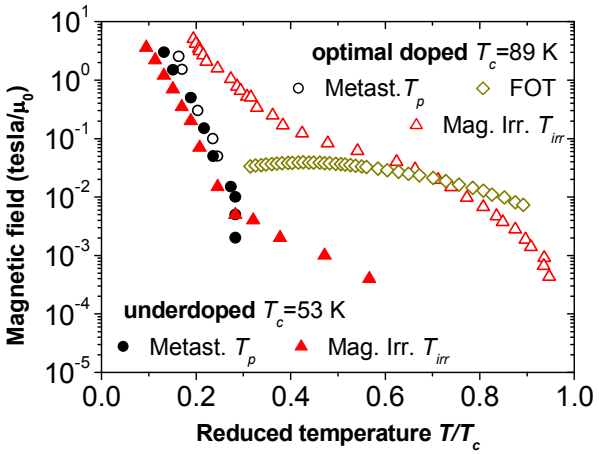


Fig.1. *Vortex (H-T) phase diagram for optimally doped and underdoped BSCCO.*

[+] Permanent position: Budapest University of Technology and Economics

[#] Ph.D. student

the glass transition temperature, but continue to explore disorder configurations into the glass phase.

Nuclear magnetic resonance in rotor – stator compounds. — We have investigated the rotor-stator molecular crystal $C_{60}{\cdot}C_8H_8$ by ^1H nuclear magnetic resonance (NMR). The ^1H line is broad and exhibits fine structure characteristic of a multispin spectrum indicating the absence of angular reorientations of the cubane molecule C_8H_8. The temperature and field dependence of the spin-lattice relaxation rate of cubane protons is well explained in terms of field fluctuations arising from the reorientations of the fullerene (C_{60}) molecules. The low activation energy (650 K) of these reorientations indicate that the cubane molecules act as efficient bearing for the rotating fullerene molecules.

E-Mail:

György Kriza	kriza@szfki.hu
Péter Matus	matus@szfki.hu
György Mihály	mihaly@phy.bme.hu
Ágnes Pallinger	pagnes@szfki.hu
Bernadette Sas	sas@szfki.hu
F.I.B. Williams	willia@szfki.hu

Grants and international cooperations

OTKA K 62866	Collective dynamics of elastic lattices in disorder potential (F.I.B. Williams, 2006-2009)
SPEC – Saclay	Collaboration agreement with Service de Physique de L'Etat Condensé (SPEC) CEA-Saclay, France on electron crystals and nano-electronics (2005-2008)

Publications

Articles

G.1 Pallinger Á, Sas B, Pethes I, Vad* K, Williams FIB, Kriza G; Breakdown of the Bardeen-Stephen law for free flux flow in $Bi_2Sr_2CaCu_2O_{8+\delta}$; *Phys Rev B*; **78**, 104502/1-5, 2008

G.2 Bokor M, Matus P, Bánki P, Kriza G, Tompa K, Kováts É, Pekker S, Bényei* G, Jalsovszky* I; ^1H NMR spectrum and spin-lattice relaxation in $C_{60}{\cdot}C_8H_8$; *phys stat sol (b);* **245**, 2010–2012, 2008

H. METAL PHYSICS

K. Tompa, I. Bakonyi, P. Bánki, M. Bokor, J. Dégi[#], Gy. Lasanda, L. Péter, B. Tóth[#], E. Tóth-Kádár

Metal-hydrogen systems. — We have investigated hydrogen charging (discharging) processes in $Pd_{0.90}Ag_{0.10}H_x$ alloys by simultaneous hydrogen concentration and nuclear spin-spin relaxation time measurements.

Hydration of intrinsically disordered proteins. — Intrinsically disordered proteins (IDPs) carry out their functions despite their lack of well-defined 3D structures. Often, these proteins function by molecular recognition, in which structural disorder confers specific advantages, such as rapid and specific binding, the capacity of binding multiple partners, or binding promiscuity, that is, the ability to bind different partners with distinct functional outcomes. Mobile water molecules within the hydrate layer of proteins can be qualitatively and quantitatively characterized by proton free-induction decays (FIDs). IDPs are characterized by a larger hydrate layer. Determination of non-freezing (hydrate) water fraction is based on the comparison of the FID signal intensity extrapolated to $t = 0$ with that measured at a temperature where the whole sample is in liquid state. The zero-time FID signal intensity is proportional to the number of resonant nuclear spins in the sample. The protein Df31, earlier described as a histone chaperone involved in chromatin decondensation and stabilization, was among the IDPs identified in the Drosophila melanogaster proteome. The temperature dependence of the extrapolated FID and CPMG-echo train amplitude of mobile water protons of Df31 and the globular control BSA was determined (Fig. 1). There is 10-15°C difference in the melting temperature of the hydrate water for globular and intrinsically disordered proteins: hydration water melts at a lower temperature for the globular BSA (-54°C) than for the IDP Df31 (-41°C) (Fig. 1A). The temperature trend of the mobile (hydration) water concentration is characteristically different for the two kinds of proteins. The globular BSA has unfrozen hydration water well below the melting point of the hydration water for the ID Df31. The ID Df31 has much higher hydration above -30°C than the globular BSA (Fig. 1A), under the given protein concentrations. When compared the hydration curves at temperature scales shifted to have common hydration melting points, the differences between the two kinds of proteins become strikingly obvious (Fig. 1B). In our experience, these differences are indicative of the open and largely exposed character of Df31 ensured by its IDP character, which ensures binding of much more water in the hydration shell.

Phase transitions in correlated electron systems: NMR experiments. — Magnetic properties of Prussian blue analogues (PBA) involve a large variety of attractive phenomena, such as spin-glass-like, photomagnetic, piezomagnetic behavior and magnetic pole inversion. The simple face centered cubic lattice of PBA compounds is however far from being free of defects and vacancies, part of the metal ion positions are vacant, while some of them are filled with water molecules. The water content, which can be modified during synthesis, influences significantly the resultant magnetic properties of the prepared PBA. The detectable ^1H nuclei (Fig. 2A) for the compound $Ni_3[Cr(CN)_6]_2 \cdot 15H_2O$ belong to either the coordinated or the zeolitic water molecules. We suppose that they belong most probably to the nickel-coordinated water by the following reasons. (*i*) There are six such water molecules per formula unit and their relative number of 6/15 = 0.4 agrees with

[#] Ph.D. student

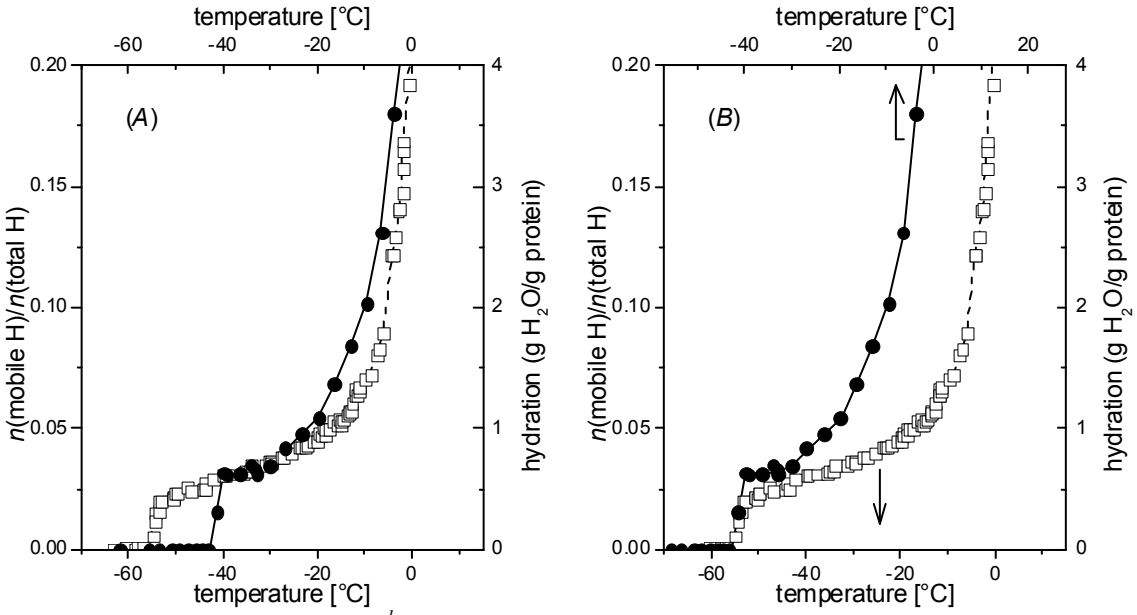


Fig. 1. *Temperature dependence of ^{1}H NMR signal intensity of Df31 (circles) and BSA (squares). Graph (A): Temperature dependence of the concentration of mobile water protons in Df31 was measured at 50 mg/mL protein concentration in water by wide-line NMR (extrapolated FID and CPMG echo-train amplitude of mobile water protons). Because the NMR amplitude is proportional to the number of protons, the intensity values yield the quantity of hydrate water below ~-5°C where the bulk water is frozen, indicating a much larger hydrate layer of the latter. Graph (B) compares the hydration curves at temperature scales shifted to have common hydration melting points. This way, the differences between the two kinds of proteins become strikingly obvious.*

the measured ratio $n_{\mathrm{NMR}}/n_{\mathrm{formula}}$. (*ii*) Much higher ratio of ^{1}H nuclei are detectable in the $x < 1$ compounds and practically all of the protons are resonant for $Mn_3[Cr(CN)_6]_2{\cdot}15H_2O$ (Fig. 2A). This can be understood if we assume that the magnetic moment of manganese ions and their magnetic interaction with chromium ions are dominant over the magnetic fields of nickel or chromium ions and over the Ni-Cr interaction. As an overall result, the protons in the manganese compounds experience more homogeneous spatial distribution of local magnetic field strength and nature than in $Ni_3[Cr(CN)_6]_2{\cdot}15H_2O$. (*iii*) The NMR parameters T_1, $T_{2\mathrm{eff}}$ and *FWHM* (Fig. 2B) show that detectable ^{1}H nuclei in the manganese containing compounds are subjects of significantly greater local magnetic moments than in $Ni_3[Cr(CN)_6]_2{\cdot}15H_2O$.

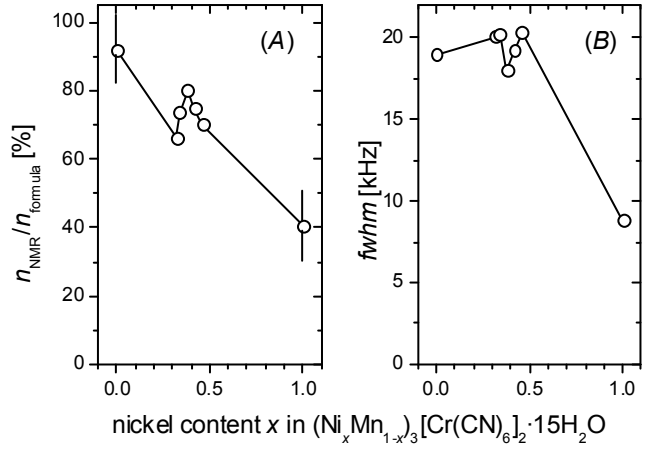


Fig. 2. *(A) NMR-detectable water content relative to the actual value corresponding to the chemical formula $(Ni_xMn_{1-x})_3[Cr(CN)_6]_2{\cdot}15H_2O$. (B) Full width at half maximum of room-temperature ^{1}H NMR spectra for $(Ni_xMn_{1-x})_3[Cr(CN)_6]_2{\cdot}15H_2O$ compounds.*

Depth profile analysis of electrodeposited multilayers. — We developed a sample preparation technique by which a new depth profile analysis method could be performed.

In all conventional depth profile analysis methods, the sputtering of the samples starts with the sample segment produced the last. In our new method, the samples were deposited onto a very smooth Si/Cr(5nm)/Cu(20nm) substrate, whose mean surface roughness is around 1 nm. After producing a metallic deposit on the substrate, the entire metallic coating can be detached from the Si wafer, and the analysis can be started from the deposit layer produced first. By this "reverse depth profiling method", the impact of the roughening of the deposit with increasing layer thickness on the depth profile analysis could be suppressed. This analysis technique also enabled us to calculate the depth profile analysis results by taking into account the development of the surface roughness that was measured with AFM for nominally identical samples. A comparison of the experimental and calculated depth profiles (Fig. 3) revealed that the deposit thickness fluctuation and the fluctuation of the individual layers within a multilayered deposit must be correlated.

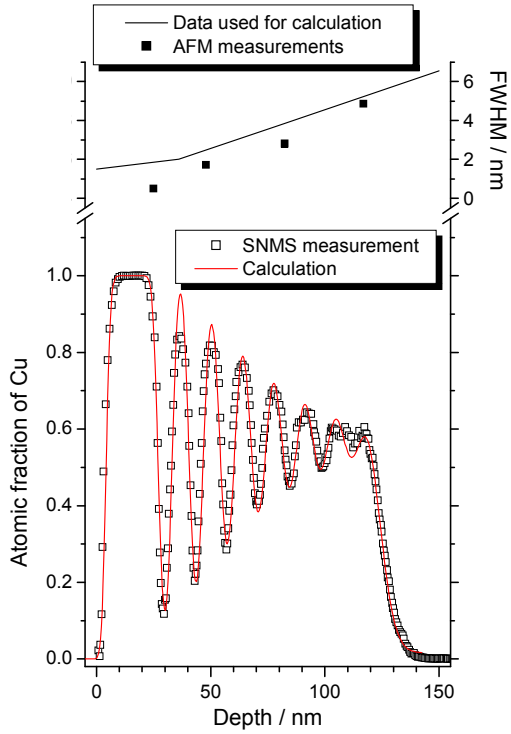


Fig. 3. *Comparison of the measured and calculated depth profile data for a multilayer sample with the following layer sequence:*

Si/Cr(5nm)/Cu(20nm)//[Co(7.0nm)/Cu(5.5nm)]X7. Secondary neutral mass spectrometry (SNMS) data were obtained in the Nuclear Research Intrutute of HAS (Debrecen, Hungary).

The top part of the figure shows the full width at half maximum (FWHM) of the measured AFM height distribution curves (symbols) and the function used for the depth profile calculation (solid line).

Magnetoresistance of electrodeposited alloys. — Co_xNi_{1-x} alloys were produced by electrodeposition in the entire composition range. The magnetoresistance of electrodeposited alloys as a function of the composition followed the trendline of the same alloy series produced by physical methods according to literature data. We have also made an attempt to deposit Cr_xNi_{1-x} alloys, but it was successful only with low chromium contents of $x<0.05$. The magnetoresistance of these alloys decreased with the chromium content, but we could not achieve the composition range where the sign of the magnetoresistance inverts according to the literature.

Structure of electrodeposited GMR multilayers. — An X-ray diffraction (XRD) study of electrodeposited Co(2.7nm)/Cu(d_{Cu}) multilayers with Cu layer thicknesses from 0.5 nm to 4.5 nm revealed that, from structural point of view, three thickness ranges can be distinguished. For $d_{Cu} < 2$ nm, a few percent of hcp-Co fraction is present and no superlattice satellite peaks can be observed. For $d_{Cu} > 2$ nm, no hcp reflections can be detected whereas clear satellite reflections appear for 2 nm $< d_{Cu} <$ 4 nm around the main fcc(111) reflection (Fig. 4, left panel). For $d_{Cu} > 4$ nm these satellite peaks can hardly be seen again. These findings can be explained by the presence of pin-holes in the Cu layers

for d_{Cu} < 2 nm, the formation of a coherent superlattice structure for 2 nm < d_{Cu} < 4 nm and the degradation of the multilayer structural quality for d_{Cu} > 4 nm. The intermediate Cu thickness range is also characterized by the strongest fcc(111) texture and by the largest structural perfectness and the XRD bilayer repeat period agreed well with the nominal values (Fig. 4, right panel). These structural data will be very helpful in explaining magnetoresistance results on the same multilayers.

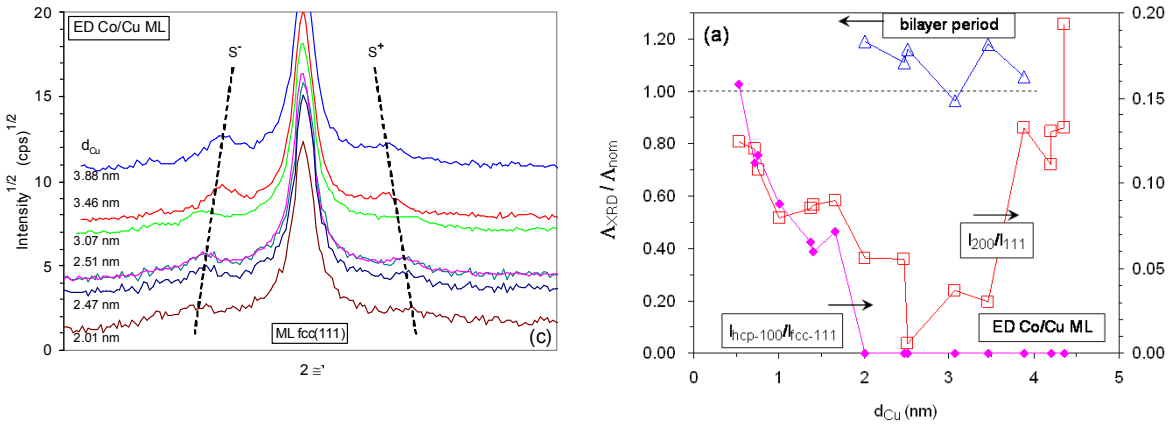


Fig. 4 *The left panel shows the XRD patterns around the (111) reflections for electrodeposited Co/Cu multilayers in the intermediate range of the Cu layer thickness (2 to 4 nm). The shift of the multilayer satellite peak positions (S^- and S^+) with varying bilayer repeat period is indicated by the dashed lines. The right panel displays for the whole Cu layer thickness range investigated the bilayer repeat period derived from the satellite peak positions and normalized with the nominal repeat period, the ratio of the hcp-Co peak intensity to the main fcc-(111) peak intensity and the ratio of the fcc-(200) and fcc-(111) peak intensities.*

E-Mail:

Imre Bakonyi	bakonyi@szfki.hu
Péter Bánki	banki@szfki.hu
Mónika Bokor	mbokor@szfki.hu
Júlia Dégi	degi@szfki.hu
György Lasanda	lasi@szfki.hu
László Péter	lpeter@szfki.hu
Kálmán Tompa	tompa@szfki.hu
Bence Tóth	tothb@szfki.hu
Enikő Tóth-Kádár	tke@szfki.hu

Grants and international cooperations

OTKA K 060 821 Investigation of deposits and nanostructures prepared by controlled precisional electrodeposition (L. Péter, 2006-2008)

OTKA T 047 094 Coupling, anisotropy and domain phenomena in magentic thin films (project leader: D.L. Nagy, MTA KFKI RMKI; SZFKI participant: I. Bakonyi, 2004-2008)

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; Metal Physics participant: M. Bokor; 2006-2009)

Long term visitor

— J.M. Garcia Torres, University of Barcelona, Spain; Feb. 15 - June 15, 2008 (Fellowship of the Catalonian Government, Spain, hosts: I. Bakonyi and L. Péter)

Publications

Articles

H.1. I. Bakonyi, L. Péter, Z.E. Horváth*, J. Pádár, L. Pogány and G. Molnár*: Evolution of structure with spacer layer thickness in electrodeposited Co/Cu multilayers. *J Electrochem Soc;* **155**, D688-D692, 2008

H.2. Bokor M, Tompa K, Kiss LF, Zentková* M, Zentko* A, Mihalik* M, Maťaš* S, Mitróová* Z; ^{1}H NMR on $(Ni_xMn_{1-x})_3[Cr(CN)_6]_2{\cdot}nH_2O$; *Acta Physica Polonica A;* **113**, 485-488, 2008

H.3. Katona* GL, Berényi* Z, Péter L, Vad* K; Depth profile analysis of electrodeposited nanoscale multilayers by SNMS; *Vacuum;* **82**, 270-273, 2008

H.4. Lasanda G, Bánki P, Bokor M, Tompa K; ^{1}H NMR spectra and echoes in Pd-H and Pd-Ag-H alloys; *J All Comp*; **450**, 22-27, 2008

H.5. Szőllősi* E, Bokor M, Bodor* A, Perczel* A, Klement* É, Medzihradszky* KF, Tompa K, Tompa* P; Intrinsic structural disorder of DF31, a Drosophila protein of chromatin decondensation and remodeling activities; *J Proteome Res;* **7**, 2291-2299, 2008

H.6. 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*; accepted for publication

H.7. Tompa K, Bánki P, Bokor M, Kamasa P, Lasanda G, Tompa* P; Interfacial water at protein surfaces: wide-line NMR and DSC characterization of hydration in ubiquitin solutions. 1; *Biophysical Journal*; accepted for publication

Book chapter

H.8. Péter L, Bakonyi I; In: *Nanomagnetism and Spintronics: Fabrication, Materials and Characterization, and Applications*; Eds.: Nasirpouri F and Nogaret A, World Scientific, Singapore; accepted for publication

Others

H.9. Bakonyi I, Simon* E, Péter L; Az óriás mágneses ellenállás felfedezése (1988) – A spintronika nyitánya – a 2007. évi fizikai Nobel-díj és háttere (The discovery of giant magnetoresistance (1988) – An overture to spintronics – The Nobel Prize in Physics 2007 and its background, in Hungarian); *Fizikai Szemle*; **58**, 41-45, 2008

H.10. Bakonyi I, Simon* E, Péter L; Mágneses ellenállás ferromágneses fémekben és mágneses nanoszerkezetekben (Magnetoresistance in feromagnetic metals and magnetic nanostructures, in Hungarian); *Fizikai Szemle*; **58**, 93-98, 2008

See also: D.3., G.2.

I. METALLURGY AND MAGNETISM

L.K. Varga, I. Balogh, É. Fazakas[#], P. Kamasa, G. Konczos, Gy. Kovács[+], J. Pádár, L. Pogány, F.I. Tóth

Metallurgy: The bulk glass forming ability (BGFA) of simple binary $Cu_{100-x}Zr_x$ (x in the range 34-40 at.%) based alloys was investigated in collaboration with the Institute for Metal Science "Acad A. Balevski", Bulgarian Academy of Sciences. The fragility parameter, m of Angell has been determined by DSC and TMS measurements and a minimum of m was found around the composition $Cu_{64}Zr_{36}$ where the formation of bulk binary metallic glass can be reached.

A new, Al based amorphous alloy free of rare-earth metals was prepared by the melt-spinning technique under protective atmosphere. The alloy $Al_{85}Ni_9Ta_6$ easily forms a ductile glass, with the crystallization onset temperature T_x = 370 ^oC, enthalpy of transformation ΔH = 68 J/g, activation energy of crystallization 2.76 eV and presenting a wide supercooled liquid region of about 58 K. The Vickers microhardness $HV_{0.01}$ = 486 is one of the biggest among the known Al-based glasses, permitting to estimate a record value of the tensile strength which makes this new glass a prospective material for preparing bulk samples by different powder consolidation techniques.

The structure of rapidly quenched $Al_{88}Fe_5Y_7$, $Al_{88}Fe_4Y_7Sb_1$ and $Al_{93}Fe_5Sb_2$ alloys was studied using XRD and Mössbauer spetroscopy. The results show that the addition of Sb affects adversely the glass forming ability of the alloy, but increases its mechanical strength. The X-ray amorphous $Al_{88}Fe_5Y_7$ alloy shows a short range order resembling that of the Al_6Fe compound as it can be judged from the Mössbauer data.

A new light-weight multi-component high-entropy alloy (MHA) was prepared ($Al_{20}Ti_{20}Zr_{20}Be_{20}Cu_{20}$), by vacuum casting in copper mould. These MHAs are expected to be one of the emerging structural materials, which are designed by the strategy of low enthalpy of mixing of the elements and equal/near-equal atomic ratio of the components conferring high entropy of mixing. The resulting low free energy keeps the structure in one phase (bcc or fcc) solid solution which possesses excellent mechanical properties as high strength and high plasticity.

Soft magnetic nanocrystalline alloys. — Induced magnetic anisotropy in Co-doped Finemet-type nanocrystalline materials has been studied using a home-made furnace with longitudinal (~ 2 kA/m) and transversal (~160 kA/m) magnetic fields applicable during the heat treatment. Flattening down to an effective permeability of 800 could be obtained with linear hysteresis loop.

The DC hysteresis loss of minor loops has been determined using a Quasi-DC hysterograph purchased through a grant of Hungarian Government (GVOP-3.2.1.-2004-04-0281/3.0). The data were analysed by Steinmetz type scaling power–laws for three different soft magnetic materials: round type Finemet, non-oriented Fe-Si sheets and Mn-Zn ferrite cores. It has been shown, by using the hyperbolic model of hysteresis, that the Steinmetz formula for calculating hysteresis losses is fully justified.

Thermal, thermomagnetic and thermomechanical testing of amorphous alloys. — A new home-built equipment was developed for high heating rate DTA measurements and is under experimental testing for Al-Ti based amorphous and nanocrystalline alloys. A

[#] Ph.D. student

[+] Permanent position: Loránd Eötvös University, Budapest

controlled heating rate as high as q = 2500 K/min can be achieved up to 800 ^{o}C. It was demonstrated that the Kissinger plot is valid up to a certain heating rate only. From the shift of crystallization (T_x) and glass transition (T_g) temperatures as a function of ln(q) two intersecting linear plots can be obtained and from their intersection, the Kauzmann temperature can be estimated.

E-Mail

István Balogh	ibalogh@szfki.hu
Éva Fazakas	efazakas@szfki.hu
Pawel Kamasa	kamasa@szfki.hu
Géza Konczos	konczos@szfki.hu
György Kovács	kovacsgy@ludens.elte.hu
József Pádár	padar@szfki.hu
Lajos Pogány	pogany@szfki.hu
Ferenc I. Tóth	ftoth@szfki.hu
Lajos K. Varga	varga@szfki.hu

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 (2008-2011, Project leader: L.K. Varga)

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, 2006-2008)

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 thermophysical 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, 2008)

Publications

Articles

I.1. Fazakas E, Varga LK; Glass-forming ability (GFA) of Cu and Al based alloys by melt-quenching; *J Mater Sci Technol (Bulgaria)*; **15**, 211-224, 2007

I.2. Bednarčík* J, Kováč* J, Roth* S, Füzer* J, Kollár* P, Varga LK, Franz* H; The soft magnetic properties and temperature stability of Co-Fe-Zr-B metallic glasses; *Acta Physica Polonica A;* **113**, 83-86, 2008

I.3. Celegato* F, Coïsson* M, Kane* SN, Mazaleyrat* F, Modak* SS, Tiberto* P, Varga LK, Vinai* F; Effect of annealing on magnetic and magnetotransport properties of $Fe_{84}Zr_{3.5}Nb_{3.5}Cu_1B_8$ ribbons; *phys stat sol (a);* **205**, 1749-1752, 2008

I.4. Fazakas É, Varga LK; Al-U based amorphous alloys obtained by melt spinning method; *Rev Adv Mater Sci.* **18**, 494-496, 2008

I.5. Justin Joseyphus* R, Narayanasamy* A, Varga LK, Jeyadevan* B; Studies on the exchange and dipolar couplings in $Nd_2Fe_{14}B/\alpha$-Fe; *Int J Mater Res*; **99**, 70-74, 2008

I.6. Kane* SN, Khinchi* SS, Gercsi* Zs, Gupta* A, Varga LK, Mazaleyrat* F; Structural studies of stress annealed $Co_{21}Fe_{64-x}Nb_xB_{15}$ alloys; *Rev Adv Mater Sci;* **18**, 572-575, 2008

I.7. Kolano* R, Kolano-Burian* A, Varga LK, Szynowski* J, Polak* M; Co added FINEMET and NANOPERM alloys with flat hysteresis loops; *Rev Adv Mater Sci;* **18**, 557-560, 2008

I.8. Kolano-Burian* A, Kolano* R, Szynowski* J, Varga LK; Induced magnetic anisotropy in Co-doped Finemet-type nanocrystalline materials; *J Magn Magn Mater;* **320**, e758-e761, 2008

I.9. Modak* SS, Ghodke* N, Mazaleyrat* F, Lo Bue* M, Varga LK, Gupta* A, Kane* SN; Structural and magnetic investigation of gradually devitrified Nanoperm alloys; *J Magn Magn Mater;* **320**, e828-e832; 2008

I.10. Nagy* E, Janovszky* D, Svéda* M, Tomolya* K, Varga LK, Sólyom* J, Roósz* A; Investigation of crystallization in an amorphous Cu-based alloy by X-ray; *Mater Sci Forum;* **589**, 131-136, 2008

I.11. Szynowski* J, Kolano* R, Kolano-Burian* A, Varga LK; Dynamic magnetic properties of the Fe-based alloys under non-sinusoidal excitation; *J Magn Magn Mater;* **320**, e841-e843, 2008

I.12. Takács* J, Kovács Gy, Varga LK; Decomposition of the hysteresis loops of nanocrystalline alloys below and above the decoupling temperature; *J Magn Magn Mater;* **320**, e1016-e1019, 2008

I.13. Takács* J, Kovács Gy, Varga LK; Hysteresis reversal; *Physica B;* **403**, 2293-2297, 2008

I.14. Varga* B, Fazakas E, Varga LK; Preparation of nanocrystalline $Al_{100-x}Si_x$ ($6 < x < 40$) based alloys by rapid solidification methods; *Metallurgia International*; **13**, 41-44, 2008

I.15. Varga LK, Davies* HA; Challenges in optimizing the magnetic properties of bulk soft magnetic materials (panel discussion); *J Magn Magn Mater;* **320**, 2411-2422, 2008

I.16. Varga LK, Kovács Gy; Separation of magnetization loop in domain wall movement and domain rotation contributions for soft magnetic materials; *Acta Physica Polonica A;* **113**, 159-162, 2008

I.17. Varga LK, Kovács Gy, Takács* J; Anhysteretic and biased first magnetization curves for Finemet-type toroidal samples; *J Magn Magn Mater;* **320**, e814-e818, 2008

I.18. Varga LK, Kovács Gy, Takács* J; Modeling the overlapping, simultaneous magnetization processes in ultrasoft nanocrystalline alloys; *J Magn Magn Mater*; **320**, L26-L29, 2008

I.19. Kamasa P, Varga LK, Myslinski* P, Rassolov* SG, Maksimov* V, Idzikowski* B; Crystallization of amorphous Fe–Cr–B alloys investigated with high heating rates; *Materials Science-Poland*; **26**, 947-952, 2008

See also: H.1., H.7.

J. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

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

Structure of condensed matter. — Bioactive glass-ceramics and composites have been successfully used for the repair, reconstruction, and replacement of diseased or damaged parts of the body, especially bones. The aim of our study was to prepare a bulk calcium silicate system that exhibits suitable properties to be used for biomedical applications. Glass-ceramics of composition $CaO{\cdot}SiO_2$ were produced by sol-gel technique starting from tetraethoxysilane and calcium nitrate tetrahydrate as well as by melt-quenching technique using a mixture of $CaCO_3$ and SiO_2. The traditional power technology requires 1500 °C temperature to produce ceramic bulks; contrarily the sol-gel technique 700 °C. Their structures were compared by means of thermo-analysis, X-ray diffraction, small angle X-ray and neutron scattering. The compactness of these materials is the key feature for biocompatibility, in this respect Small angle neutron scattering (SANS) measurements revealed important information on the temperature dependence of the fractal structure in various stages of the sample preparation. In the melt-quenched samples, the crystalline feature is dominated; the gel-derived samples are rather amorphous. The mechanical property of the calcium silicate materials obtained by different preparation routes were characterized by Brinell-hardness tests. The melt-quenching technology yields the glass-ceramics product with good mechanical strength at 1500 °C; while the gel derived products achieve this mechanical strength already after a heat treatment at 700 °C. The gel derived product prepared with ammonia catalyst proved to be the hardest and most compact matter.

Applied research with neutrons – Structural features of H_2-containing catalysts. — The presence of hydrogen determines the activity of ZnOCuH(D) catalysts, widely used for methanol synthesis, however, the catalysis mechanism governed by hydrogen behavior inside and on the surface of copper inclusions (clusters) in the ZnO matrix remains unclear. The aim of this work is to determine Cu ordering at atomic and nano-scale level as well as the location and arrangement of hydrogen atoms in the structure, related to possible influence on catalytic activity. We prepared pairs of isotopic samples $Zn_{0.92}{}^{63}Cu_{0.08}O(H)$, $Zn_{0.92}{}^{63}Cu_{0.08}O(D)$, $Zn_{0.92}{}^{65}Cu_{0.08}O(H)$ and $Zn_{0.92}{}^{65}Cu_{0.08}O(D)$, characterized by contrast according to the amplitudes of scattering on H, D, ^{63}Cu and ^{65}Cu isotopes. The migration and condensation of hydrogen in the vicinity and inside nanosized defects in the CuH(D)ZnO catalyst powders were investigated by using small-angle neutron scattering. We have obtained that the inclusions at the surface of ZnO particles and inside ZnO matrix have a complex structure: a hydrogen-rich core with radius ~4 nm is located in the center of the Cu cluster, surrounded by a hydrogen shell with external radius ~14 nm. The characteristic H(D) concentration in the core is ~15 % at., while in the shell only ~1 % at. with respect to metallic copper (Cu ~$8.5x10^{22}cm^{-3}$). The integral ratio on cluster volume of

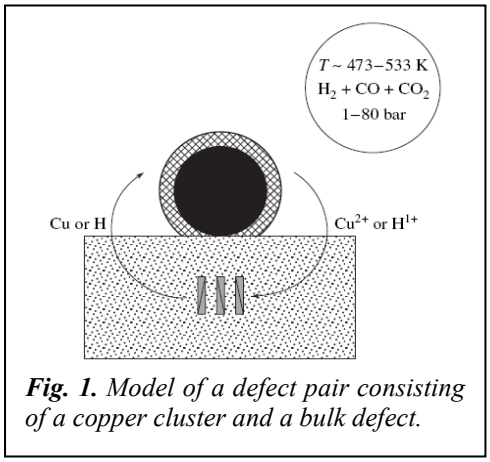


Fig. 1. *Model of a defect pair consisting of a copper cluster and a bulk defect.*

[#] Ph.D. student

number of atoms is H(D) : Cu = 1 : 10. From the calculated correlation functions the hydrogen distribution model is the following: hydrogen occupies two different positions: (i) near the defects in the ZnO matrix volume and (ii) on the surface of a defect near a copper cluster (Fig.1). These two coupled defects can form an electrochemical pair and cause a Cu – H exchange, effective direction of which depends on the composition and temperature of the gas medium, where the catalyst is placed. Such pairs assist the decomposition of molecular hydrogen into atomic hydrogen involved in the methanol synthesis reaction.

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 serve for basic and applied research as well as for instrument development. Recently a new record in quasielastic neutron scattering spectroscopy was reached with substantial contribution from our Laboratory. As a part of our current instrument development project (NAP 2005-08) in the frame of our partnership with the Institute Laue-Langevin (ILL, Grenoble) this result was achieved on the IN15 neutron spin echo (NSE) spectrometer at ILL with the participation of our scientists.

In quasielastic neutron scattering highest energy resolution measurements can be achieved by NSE method invented by F. Mezei still in 1972. This technique uses the Larmor precession of the neutrons to avoid the usual phase space problem of conventional energy analysis what appears in other methods such as in time-of-flight (TOF) or triple axis spectrometry whereas for the better resolution one need better monochromatization what yields less neutron luminosity. The first spin-echo spectrometer ever built is the IN11 instrument at the ILL; on this device the 50 ns time-resolution became routinely usable at reasonable intensities in the past few decades.

The next step in energy resolution was the construction of the IN15 at the new cold source of ILL. The key issue in time/energy resolution is the Larmor precession guide field inhomogeneities, so, for higher resolution more correction coils (Fresnel-lenses) have to be applied i.e. more material has to be inserted in the beam, again reducing luminosity especially at the very long wavelength range. With conventional correction coils (Cu-foils) 100 ns became available routinely (in 1997, Schleger, Ehlers et al). To “tune up this instrument” one has to optimize about 20-30 current in different coils and about 10 mechanical positions, while the problem of scattering and absorption of these correction devices placed in the beam requires special attention.

These two problems had been solved by the methods developed and correction coils designed by us. The new correction coils – self-sustaining thin Al-foil structure – were manufactured in Hungary. Using these coils a part of the correction system of IN15 had been replaced recently and the 1μs correlation time had been reached. Our contribution to this development (in theory, technology, and manufacturing) is utmost significant, since many new spin-echo instruments are planned to be built or are already under construction world-wide, thus a major component of these devices can be realized with this new technology.

E-Mail:

László Rosta rosta@szfki.hu
László Almásy almasy@sunserv.kfki.hu
László Cser cser@sunserv.kfki.hu
Irina Gladkih gladkih@sunserv.kfki.hu

István Füzesy	fuzesy@szfki.hu
János Füzi	fuzi@sunserv.kfki.hu
György Káli	kali@szfki.hu
Tibor Kun	kunt@szfki.hu
Adél Len	lenadel@sunserv.kfki.hu
Márton Markó	marko@szfki.hu
Anikó Meiszterics	meiszterics@sunserv.kfki.hu
Ferenc Mezei	mezei@lanl.gov
Gergely Nagy	nature.elatus@gmail.com
János Orbán	orban@szfki.hu
Eszter Rétfalvi	retfalvi@sunserv.kfki.hu
Zsombor Sánta	santa@szfki.hu
Noémi Kinga Székely	szekely@szfki.hu
Gyula Török	torok@szfki.hu
Tamás Veres	vertam@freemail.hu

Grants and international cooperations

EU HII3-CT-2003-505925 Access to Research Infrastructure (BNC, L. Rosta, 2004-2008)

EU HII3-CT-2003-505925 JRA2 Detector development project (L. Rosta, 2004-2008)

EU HII3-CT-2003-505925 JRA3 Focusing neutron optics project (J. Füzi, 2004-2008)

EU HII3-CT-2003-505925 JRA2 Polarised neutron techniques (Gy.Török, 2004-2008)

IAEA-13507 Improvement of neutron beam performance and sample environment in residual stress (Gy. Török, 2006-2008)

OM-00079/2008 (Jedlik) Research and development of marketable materials and technologies for neutron instrumentation (J. Füzi, 2008-2011)

NAP VENEUS-2005 OMFB-00648/2005 Visegrad cooperation for development and application of neutron spectroscopy techniques in multidisciplinary research (L. Rosta, 2005-2008)

TET UKR-2006 Nanotubes (L. Rosta, 2007-2008)

Long-term visitors

— Prof Bo Chen and Mr Jianming Song, Institute of Nuclear Physics and Chemistry, China Academy of Engineering Physics, Sichuan, PR China, October 25 - December 10, 2008 (host: L Rosta)

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

— Dr Mikhail Avdeev, Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research Dubna, Russia, August 19 - September 18, 2008 (host: L Rosta)

— Sergey Kozhevnikov, Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research Dubna, Russia, September 9 - October 6, 2008 (host: L Rosta)

— Gerard Pépy, Epinay-sur-Orge, France, August 17 - September 15 and November 3-17, 2008 (host: L Rosta)

Publications

Articles

J.1. Cser L, Krexner* G, Marko M, Sharkov* I, Török Gy; Neutron holography; *Acta Phys Hung B*; **26**, 189–194, 2006

J.2. Mykhaylyk* OM, Kotsuruba* AV, Dudchenko* NO, Török Gy; Some signal effects in human erythrocytes on specific binding of free doxorubicin and doxorubicin conjugates with magnetite nanoparticles; *Ukrainskii Biokhimicheskii Zhurnal*; **77**, 84-92, 2006

J.3. Kulvelis* YV, Lebedev* VT, Török Gy, Melnikov* AB; Structure of the water salt solutions of DNA with sulfonated scandium diphthalocyanine; *Journal of Structural Chemistry*; **48**, 740-746, 2007

J.4. Lebedev* VT, Vinogradova* LV, Török Gy; Structural features of star shaped fullerene (C60) containing polystyrenes: Neutron scattering experiments; *Polymer Science Ser A*; **50,** 1090-1097, 2007

J.5. Almásy L, Turmine* M, Perera* A; Structure of aqueous solutions of ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate by small-angle neutron scattering; *Journal of Physical Chemistry B*; **112**, 2382-2387, 2008

J.6. Füzi J; Direct measurement of cold neutron moderator spectra; *Nuclear Instruments and Methods in Physics Research A*; **586**, 41-45 2008

J.7. Füzi J; Quality assessment of in-pile guides by energy resolved neutron imaging; *Nuclear Instruments and Methods in Physics Research A*; **586**. 46-50, 2008

J.8. Füzi J; Neutron motion in magnetic fields; *Meas Sci & Techn*; **19**, 034013/1-6, 2008

J.9. Füzi J; Spectral accuracy of multiwire proportional counter detectors in time of flight regime; *Meas Sci & Techn*; **19**, 034028/1-7, 2008

J.10. Hanski* S, Junnila* S, Almásy L, Ruokolainen* J, Ikkala* O: Structural and conformational transformations in self-assembled polypeptide-surfactant complexes; *Macromolecules*; **41**, 866-872, 2008

J.11. Heaton* ME, Rogante* M, Len A; A feasibility study for a SANS investigation of a heat cured and laser machined organic resin microturbine as used for airflow sensing; *Multidiscipline Modeling in Materials and Structures*, **4**, 155-162, 2008

J.12. Knaapila* M, Almásy L, Garamus* VM, Ramos* ML, Justino* LLG, Galbrecht* F, Preis* E, Scherf* U, Burrows* HD, Monkman* AP; An effect of side chain length on the solution structure of poly(9,9-dialkylfluorene)s in toluene; *Polymer*; **49,** 2033-2038, 2008

J.13. Kyzyma* OA, Bulavin* LA, Aksenov* VL, Avdeev* MV, Tropin* TV, Korobov* MV, Snegir* SV, Rosta L; Organization of fullerene clusters in the system C60/N-methyl-2-pyrrolidone; *Materials structure*; **15**, 17−20, 2008

J.14. Kyzyma* OA, Bulavin* LA, Aksenov* VL, Tropin* TV, Avdeev* MV, Korobov* MV, Snegir* SV, Rosta L; Aggregation in C60/NMP, C60/NMP/water and C60/NMP/toluene mixtures; *Fullerenes, Nanotubes and Carbon Nanostructures*; **16**, 610–615, 2008

J.15. Lebedev* VT, Török Gy, Melenevskaya* EY, Vinogradova* LV, Ivanova* IN; Poly(N-vinylcaprolactam)-C60 complexes in aqueous solution; *Fullerenes, Nanotubes and Carbon Nanostructures*; **16**, 603 – 609, 2008

J.16. Meiszterics A, Sinkó* K; Calcium silicate ceramics; *Colloids and Surfaces A: Physico-chemical and Engineering Aspects*; **319**, 143-148, 2008

J.17. Petrenko* VI, Bulavin* LA, Avdeev* MV, Aksenov* VL, Rosta L; Neutron investigations of the interaction of surfactant molecules in non-polar solvent; *Ukrainian Journal of Physics*; **53**, 229-233, 2008

J.18. Petrenko* VI, Bulavin* LA, Avdeev* MV, Aksenov* VL, Rosta L; Neutron investigations of magnetite-oleic acid-benzene ferrofluids stability with the excess of surfactant (in Ukrainian); *Journal of Physical Studies*; **12**, 3201-3204, 2008

J.19. Rosta L, Füzi J, Török Gy; Design of focusing SANS spectrometer at BNC; *Meas Sci & Techn*; **19**, 034008/1-5, 2008

J.20. Sinkó* K, Meiszterics A, Rosta L; Comparative study of calcium silicate bulk systems produced by different methods; *Progress in Colloid and Polymer Science*; **135**, 130–138, 2008

J.21. Vass* Sz, Pedersen* JS, Plestil* J, Laggner* P, Rétfalvi E, Varga* I, Gilányi* T; Ambiguity in determining the shape of alkali alkyl sulfate micelles from small-angle scattering data; *Langmuir*; **24**, 408-417, 2008

J.22. Bende* A, Almásy L; Weak intermolecular bonding in N,N'-dimethylethyleneurea dimers and N,N'-dimethylethyleneurea – water systems: The role of the dispersion effects in intermolecular interaction; *Chemical Physics*; **354**, 202-210, 2008

J.23. Koszor* O, Tapasztó* L, Markó M, Balázsi* Cs; Characterizing the global dispersion of carbon nanotubes in ceramic matrix nanocomposites; *Appl Phys Lett*; **93**, 201910/1-3, 2008

J.24. Aksenov* VL, Tropin* TV, Kyzyma* OA, Avdeev* MV, Korobov* MV, Rosta L; On fullerene cluster formation in nitrogen-containing solvents; *Physics of the Solid State*; accepted for publication

J.25. Avdeev* MV, Bica* D, Vekas* L, Aksenov* VL, Feoktystov* AV, Rosta L, Garamus* VM, Willumeit* R; Structural aspects of stabilization of magnetic fluids by mono-carboxylic acids; *Advanced Materials Research*; accepted for publication

J.26. Avdeev* MV, Tropin* TV, Aksenov* VL, Rosta L, Kholmurodov* MT; On fullerene cluster formation in carbon disulfide. Data of small-angle neutron scattering and molecular dynamic simulation; *Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques*; accepted for publication

J.27. Barna* IF, Imre* AR, Rosta L, Mezei F; Two-phase flow model for energetic proton beam induced pressure waves in mercury target systems in the planned European Spallation Source; *EPJ B Condensed Matter and Complex Systems*; accepted for publication

J.28. Bende* A, Almásy L; Weak intermolecular bonding in N,N'-dimethylethyleneurea dimers and N,N'-dimethylethyleneurea – water systems: The role of the dispersion effects in intermolecular interaction; *Chemical Physics*; accepted for publication

J.29. Feoktystov* AV, Avdeev* MV, Aksenov* VL, Bulavin* LA, Bica* D, Vekas* L, Garamus* VM, Willumeit* R; Contrast variation in small-angle neutron scattering from magnetic fluid magnetite/myristic acid/benzene; *Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques*; accepted for publication

J.30. Gomes* SR, Margaca* FMA, Miranda Salvado* IM, Falcao* AN, Almásy L, Teixeira* J; SANS investigation of PDMS hybrid materials prepared by gamma-irradiation; *Nuclear Instruments and Methods in Physics Research Section B*; accepted for publication

J.31. Knaapila* M, Garamus* VM, Almásy L, Pang* JS, Forster* M, Gutacker* A, Scherf* U, Monkman* AP; Fractal aggregates of polyfluorene-polyaniline triblock copolymer in solution state; *J Phys Chem B*; accepted for publication

J.32. Kulvelis* YV, Trunova* VA, Lebedev* VT, Orlova* DN, Török Gy, Gelfond* ML; Synthesis and structural study of ferrofluid complexes with photodithazine and their application in PDT; *Journal of Polymer Physics*; accepted for publication

J.33. Markó M, Cser L, Krexner* G, Török Gy; Theoretical consideration of the optimal performance of atomic resolution holography; *Meas Sci & Techn*; accepted for publication

J.34. Petrenko* VI, Aksenov* VL, Avdeev* MV, Bulavin* LA, Rosta L, Vekas* L, Garamus* VM, Willumeit* R; Structure analysis of water-based ferrofluids by means of small-angle neutron scattering; *Physics of the Solid State*; accepted for publication

J.35. Petrenko* VI, Avdeev* MV, Aksenov* VL, Bulavin* LA, Rosta L; Effect of surfactant excess in non-polar ferrofluids probed by small-angle neutron scattering; *Advanced Materials Research*; accepted for publication

J.36. Petrenko* VI, Avdeev* MV, Aksenov* VL, Bulavin* LA, Rosta L; Magnetic fluids with the excess of surfactants. Data of small-angle neutron scattering, *Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques*; accepted for publication

J.37. Petrenko* VI, Avdeev* MV, Almásy L, Bulavin* LA, Aksenov* VL, Rosta L, Garamus* VM; Interaction of mono-carboxylic acids in benzene by small-angle neutron scattering; *Colloids and Surfaces A*, accepted for publication

J.38. Savii* C, Almásy L, Ionescu* C, Székely NK, Enache* C, Popovici* M, Sora* I, Nicoara* D, Savii* GG, Susan Resiga* D, Subrt* J, Stengl* V; Mesoporous silica

matrices derived from sol-gel process assisted by low power ultrasonic activation; *Processing and Application of Ceramics*; accepted for publication

J.39. Székely NK, Jancsó* G; Small-Angle Neutron scattering and volumetric studies of dilute solutions of N,N'-dimethylpropyleneurea in heavy water; *J Phys Chem*; accepted for publication

J.40. Várkonyi* Zs, Nagy G, Lambrev* PH, Kiss* AZ, Székely N, Rosta L, Garab* Gy; Effect of phosphorylation on the thermal- and light-stability of the thylakoid membranes; *Photosynthesis Research*; accepted for publication

Conference proceeding

J.41. Rosta L; Neutron research for materials science and nanotechnology at the Budapest Neutron Centre, In: *Proc of 1st Italian Workshop for Industry "Industrial Applications of Neutron Techniques", Italy, 12-14 June, 2008;* organised by Rogante Engineering, Civitanova Marche; accepted for publication

Book chapters

J.42. Füzi J; Neutron beam phase space mapping, In: *Modern Developments in X-Ray and Neutron Optics*; Eds.: Erko A, Krist Th, Idir M, Michette AG, Springer; 43-57, 2008

J.43. Krist* Th, Teichert* A, Kovács-Mezei* R, Rosta L; Neutron supermirror development, In: *Modern Developments in X-Ray and Neutron Optics*; Eds.: Erko A, Krist Th, Idir M, Michette AG, Springer; pp. 355-370, 2008

K. NEUTRON SCATTERING

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

Liquids. — Synchrotron X-ray diffraction results obtained for *liquid tin tetraiodide, SnI_4*, have been modelled by means of the reverse Monte Carlo (RMC) method. Partial radial distribution functions and distance dependent correlations between molecular orientations were determined directly from the particle coordinates. It was found that well defined orientational correlations exist beyond the first co-ordination sphere. After a debate in the literature, it was possible to establish that the correct density of the liquid is 3.7 g/cm^3. In contrast to liquids of symmetric XCl_4 molecules, the corner-to-face ('Apollo') type orientation of neighbouring molecules has a significant (about 20 % at a Sn-Sn distance of about 7 Å) weight in liquid SnI_4 (see Fig. 1). Via comparison with a reference system we demonstrated that intermolecular two-particle correlations in liquid SnI_4 are determined largely by excluded volume (steric) effects; that is, intermolecular pair interactions play only a minor role. This feature, together with the softness of the molecule, can explain the rich phase behavior of SnI_4 at high pressure.

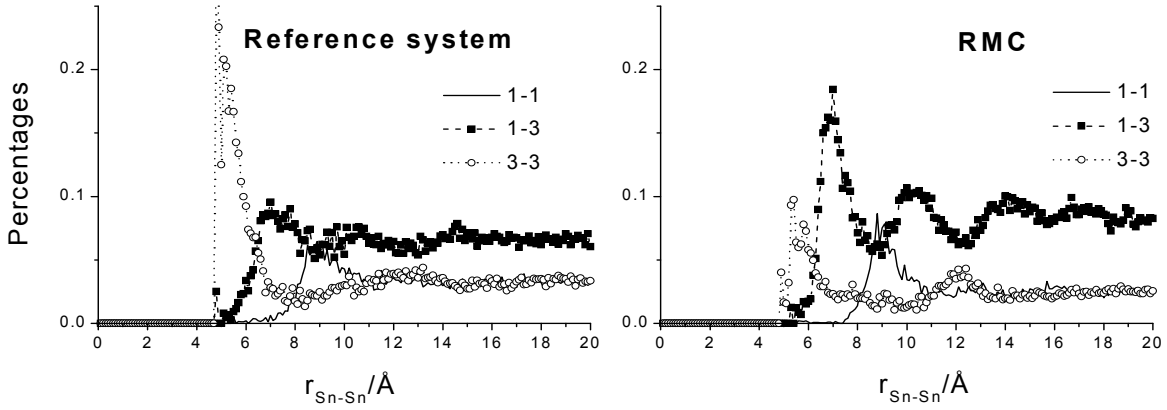


***Fig. 1**. Orientational correlation functions for liquid SnI_4, as defined by Rey [J. Chem. Phys. **126,** 164506 (2007)]. Left panel: hard-sphere-like reference system; right panel: Reverse Monte Carlo model. Solid squares denote the corner-to-face ('Apollo') type correlations. Solid line: 1:1; dashed line with solid squares: 1:3; dots with open circles: 3:3.*

X-ray diffraction results obtained for room temperature, high pressure *fluid oxygen and nitrogen, O_2 (at 0.9, 1.2, 4.3 and 5.2 GPa) and N_2, (at 2.5 GPa)*, have been interpreted via the reverse Monte Carlo method. Site-site and center-center radial distribution functions, as well as distance dependent orientational correlations have been determined by using Reverse Monte Carlo modelling. It could be established that well defined orientational correlations exist in all of the materials, particularly below about 3.5 Å. In agreement with *ab initio* molecular dynamics (MD) simulations, the dominant mutual arrangement of O_2 molecules appears to be the parallel one; here, however, the importance of X shaped and (for the higher density oxygen sample, at larger intermolecular distances) chainlike alignments has also been revealed.

Chalcogenide glasses. — *As_xTe_{100-x} glasses* ($20 \leq x \leq 60$) were studied by high energy X-ray diffraction, neutron diffraction, and EXAFS measurements at the As- and Te- K edges. The reverse Monte Carlo simulation technique was used to generate large scale models

[#] Ph.D. student

compatible with experimental data. Analysis of the resulting atomic configurations revealed that homonuclear bonding is important over the whole glass forming region. At the stoichiometric composition ($As_{40}Te_{60}$) the average As-As and Te-Te coordination numbers amount to 1.7±0.2 and 1.3±0.1, respectively. As-As bonding is significant in the Te-rich region (34≥x) while Te-Te bonding is considerable in the As-rich region (x≥50), as well. It has been shown that Te is predominantly twofold coordinated for x≤50 while As is threefold coordinated for all compositions investigated. It can be concluded that chemical ordering does not play an important role in the formation of short range order of As-Te glasses and – similarly to some other amorphous tellurides – (e.g. $Ge_2Sb_2Te_5$, $GeSb_2Te_4$, $As_{25}Si_{40}Te_{35}$) glassy As-Te alloys obey the '8-N' rule for x≤50.

Metallic glasses. — *Glassy $Co_{43}Fe_{20}Ta_{5.5}B_{31.5}$* exhibits the highest fracture strength (5185 MPa) and Young modulus (268 GPa) among all known bulk crystalline and glassy alloys. The structural background of the high mechanical stability has been investigated by means of neutron- and X-ray diffraction as well as EXAFS measurements at Co- and Fe K and Ta L I absorption edges. The simultaneous modelling of the five experimental datasets revealed the following main characteristic features: i) the majority of Fe/Co atoms have 1 Ta neighbour; ii) the B-B coordination number is about 2, which is significantly higher than the value (~1) found in amorphous $Ni_{65}B_{35}$; iii) the coordination number of Ta is about 15 and the composition of the average Ta first neighbour environment is very close to the metastable phase [$(Co,Fe)_{21}Ta_2B_6$] appearing slightly above T_g. From the above findings it can be inferred that the structure of the glassy state is based on some densely packed Ta-centered 'units' or 'clusters'. The high B-B coordination number can also contribute to the mechanical strength of the alloy.

Alkali borate glasses. — *Vitreous v-B_2O_3 and alkali borate glasses* are classical glass forming materials due to their several technological applications as key components in many kinds of commercial glasses. Neutron diffraction and infrared spectroscopy measurements have been performed on v-B_2O_3 and on $75B_2O_3$-$25Na_2O$ glasses synthesized by melt quench technique. Both methods indicate that addition of Na_2O converts the trigonal BO_3 units partly into tetrahedral BO_4 groups. The network structure of $75B_2O_3$-$25Na_2O$ glass consists of 58% BO_3 and 41% BO_4 with an average coordination number of $CN_{B\text{-}O}$= 3.4 atoms, as obtained by RMC simulation. The B-O first neighbour distance is located at 1.37 Å in *v*-B_2O_3, while two well resolved distances were found at 1.38 and 1.50 Å in the $75B_2O_3$-$25Na_2O$ glass. The analyses of the <O-B-O> and <B-O-B> three particle bond angle distributions show an extra peak at 90° in the $75B_2O_3$-$25Na_2O$ glass in addition to the peak at 120° characteristic for BO_3 trigonal units. All these findings suggest the formation of polyborate superstructure groups containing both BO_3 and BO_4 units. It was found for the ring size distribution in the v-B_2O_3 network, that 12% of boron atoms form boroxol groups (B_3O_3), while the fraction of 7–11 boron membered rings is 52%, and the tail of the distribution extends up to 20-membered rings (see Fig. 2).

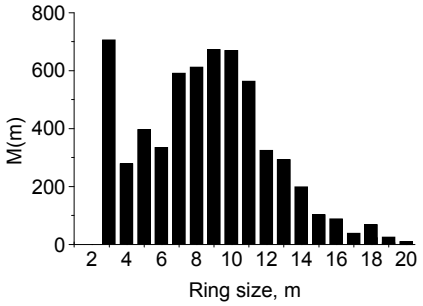


***Fig. 2**. Ring size distribution, M(m), for v-B_2O_3 as calculated from results of RMC modelling*

E-Mail:

Margit Fábián	fabian@szfki.hu
Ildikó Harsányi	harsanyi@szfki.hu
Pál Jóvári	jovari@szfki.hu
László Kőszegi	koszegi@szfki.hu
György Mészáros	meszaros@szfki.hu
Viktória Mile	milev@szfki.hu
Szilvia Pothoczki	pszzse@freemail.hu
László Pusztai	lp@szfki.hu
Erzsébet Sváb	svab@szfki.hu
László Temleitner	temla@szfki.hu

Grants and international cooperations

OTKA T 048580 Structural studies of liquids and amorphous materials by diffraction and computer modelling (L. Pusztai, 2005-2008)

OTKA IN 64279 Structural studies of liquids and amorphous materials by diffraction and computer modelling (International, with Dr. S. Kohara, Spring-8, Japan; L. Pusztai, 2006-2008)

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 HPRI-RII3-CT-2003-505925 Access to Research Infrastructure, BNC coordinated by M. Makai (neutron diffraction E. Sváb, 2004-2007)

Long term visitors

— A. Vrhovsek, University of Ljubljana, 1 September – 31 December 2008 (L. Pusztai)

Publications

Articles

K.1. Dominguez* H, Pizio* O, L. Pusztai L, Sokolowski* S; The structural properties and diffusion of a three-dimensional isotropic core-softened model fluid in disordered porous media. Molecular dynamics simulation; *Adsoprtion Science&Technology;* **25**, 479-491, 2007

K.2. Pusztai L, Pothoczki Sz, Kohara* S; Orientational correlations in molecular liquid SnI_4; *J Chem Phys*; **129**, 064509/1-4, 2008

K.3. Temleitner L, Pusztai L, Akahama* Y, Kawamura* H, Kohara* S, Ohishi* Y, Takata* M; Orientational correlations in high-pressure fluid oxygen and nitrogen; *Phys Rev B* **78**, 014205/1-6, 2008

K.4. Pusztai L, Harsányi I, Dominguez* H, Pizio* O; Assessing the level of consistency between diffraction experiments and interaction potentials: A combined molecular dynamics (MD) and Reverse Monte Carlo (RMC) approach; *Chem Phys Letts*; **457**, 96-102, 2008

K.5. Jóvári P, Kaban* I, Steiner* J, Beuneu* B, Schöps* A, Webb* A; Local order in amorphous $Ge_2Sb_2Te_5$ and $GeSb_2Te_4$; *Phys Rev B;* **77**, 035202/1-6, 2008

K.6. Fábián M, Sváb E, Proffen* Th, Veress* E; Structure study of multi-component borosilicate glasses from high-Q neutron diffraction measurement and RMC modelling; *J Non-Cryst Solids;* **354**, 3299-3307, 2008

K.7. Tzankov* D, Kovacheva* D, Krezhov* K, Puźniak* R, Wiśniewski* A, Sváb E, Mikhov* M; Magnetic properties of $Bi_{0.5}Sr_{0.5}Fe_xMn_{1-x}O_3$ ($0.1 \leq x \leq 0.7$); *J Appl Phys;* **103**, 053910/1-7, 2008

K.8. Pamukchieva* V, Szekeres* A, Sváb E, Fábian M, Révay* Z, Szentmiklósi* L; Spectral ellipsometric determination of the optical constants of multicomponent chalcogenide films of Ge-Sb-S-Te system; *J Phys: Conf. Ser*; **113**, 012054/1-5, 2008

K.9. Jóvári P, Yannopoulos* SN, Kaban* I, Kalampounias* A, Lishchynskyy* I, Beuneu* B, Kostadinova* O, Welter* E, Schöps* A; Structure of As_xTe_{100-x} ($20 \leq x \leq 60$) glasses investigated with EXAFS, X-ray and neutron diffraction and reverse Monte Carlo simulation; *J Chem Phys*; accepted for publication

K.10. Pusztai L, Dominguez* H, Pizio* O, Sokolowski* S; Detailed structural analysis of a 2 molal aqueous rubidium bromide solution: A combined molecular dynamics and Reverse Monte Carlo approach; *J Mol Liq*; accepted for publication

K.11. Pusztai L, Pizio* O, Sokolowski* S; Comparison of interaction potentials of liquid water with respect to their consistency with neutron diffraction data of pure heavy water; *J Chem Phys*; accepted for publication

K.12. Pothoczki Sz, Pusztai L; Molecular liquid $TiCl_4$ and VCl_4: two substances, one structure?; J Mol Liq; accepted for publication

K.13. Ohara* K, Kawakita* Y, Temleitner L, Pusztai L, Kohara* S, Jono* A, Shimakura* H, Inoue* N, Takeda* S; Structural analysis of lithium lanthanum titanate with perovskite structure; phys stat sol; accepted for publication

Conference proceedings

K.14. Balaskó* M, Sváb E, Kiss* Z, Tanács* A, Nagy* A, Kuba* A; Study of the inner structure of a damaged control rod by neutron-and X-ray radiography and discrete tomography; In: *Proc. of Contributed papers, 8th World Conference on Neutron Radiography, October 15-20, 2006, USA;* Ed. M.Arif & R.G.Downing, DEStech Publ. Inc. Pennsylvania, USA; pp. 294-303, 2008

K.15. Balaskó* M, Sváb E, Endrőczi* G, Tarnai* Gy, Molnár* Gy, Vigh* Z; Study of defects in helicopter rotor blade reference objects by neutron-, and X-ray radiography, vibration diagnostics and ultrasound testing; In: *Proc. of Contributed papers, 8th World Conference on Neutron Radiography, October 15-20, 2006, USA;* Ed. M.Arif & R.G.Downing, DEStech Publ.Inc. Pennsylvania, USA; pp. 304-312, 2008

Book chapter

K.16. Jóvári P, Kaban* I; Structural study of multicomponent glasses by the reverse Monte Carlo simulation technique; *Nanostructured Materials for Advanced Technological Applications*; Ed. J. P. Reithmaier, P. Petkov, W. Kulisch, C. Popov; accepted for publication

L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

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

Experimental research. — We carried on the development efforts on our unique, long-cavity Ti:sapphire oscillator which delivers orders of magnitude more pulse energy than standard, short-cavity Ti:sapphire systems. We tested novel dispersive mirrors in the cavity and demonstrated that this new multilayer design is also suitable for intracavity applications. In addition, we started to set up the acousto-optic cavity dumping of the oscillator which is expected to bring a factor of 3-4 additional enhancement in the outcoupled pulse energy.

We carried out further experimental investigations of femtosecond phenomena in surface plasmon polariton (SPP) fields. We found that the scattered light from the surface where SPPs propagate has a significantly different angular distribution when the phenomenon is induced by intense femtosecond laser pulses. The SPP–emitted light intensity shows a nonlinear dependence on that of the inducing laser light. Nonlinear frequency conversion phenomena mediated by SPPs on the surface, such as second harmonic generation and continuum spectrum generation were also observed.

In a collaboration with the Vienna University of Technology we investigated SPP enhanced electron acceleration induced by few-cycle laser pulses. Using state-of-the-art lasers in Vienna, we could demonstrate that the electrons leave the surface in 2-3 fs-long bunches. The length of the electron bunch is determined solely by the intensity envelope of the SPP generating laser pulse.

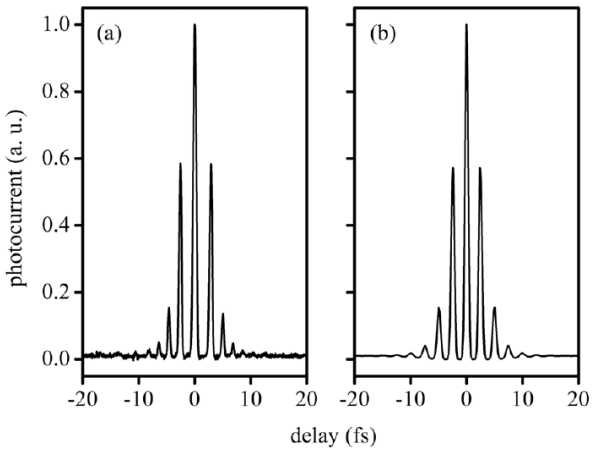


Figure 1. *Fourth order autocorrelation function of a 5-fs laser pulse (a) measured with SPP-accelerated electrons (b) calculated from the laser field.*

Theoretical research. — Our latest result in attophysics is that we have shown that the above-threshold electron de Broglie waves, generated by an intense laser pulse at a metal surface, are interfering to yield attosecond electron pulses. Owing to the inherent kinematic dispersion, the propagation of attosecond de Broglie waves in vacuum is very different from that of attosecond light pulses, which propagate without changing shape. The clean attosecond structure of the current at the immediate vicinity of the metal surface is largely degraded due to the propagation, but it partially recovers at certain distances from the surface. Accordingly, above the metal surface, there exist “collapse bands”, where the electron current is erratic or noise-like, and there exist “revival layers”, where the electron current consists of ultrashort pulses of attosecond duration.

We have also shown, based on a simple numerical model of surface plasmon enhanced electron acceleration, that it is possible to generate monoenergetic femtosecond electron bunches with this method. These results are particularly interesting for the development of

electron sources for ultrafast, high-spatial-resolution material characterization methods, such as ultrafast electron diffraction.

We investigated the correlations of detection events in two photodetectors placed at the opposite sides of a beam splitter in the frame of classical probability theory. It is assumed that there is always only one photon present in the measuring apparatus during one elementary experiment (one measurement act). Due to the conservation of energy, there is always a strict anticorrelation in one elementary experiment, because the photon cannot excite both of the detectors at the same time. It is explicitely shown in several examples that the "bunching" and "anti-bunching" of the counts in series of elementary single-photon experiments is governed by the statistical properties of grouping the sequences of the elementary measurements.

We used the exact analytic solutions of the energy eigenvalue equation of the system consisting of a free electron and one mode of the quantized radiation field for studying the physical meaning of a class of number-phase minimum uncertainty states. The states of the mode which minimize the uncertainty product of the photon number and the Susskind and Glogower cosine operator have been obtained by others. However, these states have so far been remained mere mathematical constructions without any physical significance. It is proved that the most fundamental interaction in quantum electrodynamics – namely the interaction of a free electron with a mode of the quantized radiation field – leads quite naturally to the generation of the mentioned minimum uncertainty states. It is shown that from the entangled photon-electron states developing from a highly excited number state, due to the interaction with a Gaussian electronic wave packet, the minimum uncertainty states can be constructed. In the electron's coordinate representation the physical meaning of the expansion coefficients of these states are the joint probability amplitudes of simultaneous detection of an electron and of a definite number of photons. The photon occupation probabilities in these states preserve their functional form as time elapses, but they depend on the location in space-time of the detected electron. An analysis of the entanglement entropies derived from the photon number distribution and from the electron's density operator is given.

E-Mail

Győző Farkas	farkas@szfki.hu
Péter Dombi	dombi@szfki.hu
Norbert Kroó	kroo@office.mta.hu
Miklós Lenner	lenner@szfki.hu
Péter Rácz	raczp@szfki.hu
Sándor Varró	varro@sunserv.kfki.hu, vs@szfki.hu

Grants and international cooperations

OTKA 73728 Attosecond dynamics of matter in ultra-high laser fields with sub-cycle temporal and sub-wavelength, nanometer-scale spatial resolution (S. Varró, G. Farkas, 2008-2011)

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)

ÖVEGES József Grant of the National Office for Research and Technology (P. Dombi, 2007-2008)

COST Action P 14 *"ULTRA"* Laser-matter physics with ultra-short pulses, high-frequency pulses and ultra-intense pulses. (Gy. Farkas, 2004-2008)

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)

Publications

Articles

L.1. Varró S, Farkas Gy; Attosecond electron pulses from interference of above-threshold de Broglie waves; *Laser and Part Beams;* **26**, 9-19, 2008

L.2. Dombi P, Rácz P, Ultrafast monoenergetic electron source by optical waveform control of surface plasmons; *Optics Express;* **16**, 2887, 2008; also featured as a Research Highlight in *Nature Photonics*, **2,** 206-207, 2008

L.3. Dombi P, Rácz P; Carrier-envelope phase-controlled laser-surface interactions; *Proc. SPIE*; **6892**, 68921J, 2008

L.4. Barna* IF, Dombi P; Coherent control for the spherical symmetric box potential in short and intensive XUV laser fields; *Centr Eur J Phys;* **6**, 205, 2008

L.5. Varró S; Correlations in single-photon experiments; *Fortschritte der Physik;* **56**, 91-102, 2008

L.6. Varró S; Entangled photon-electron states and the number-phase minimum uncertainty states of the photon field; *New J Phys;* **10**, 053028/1-35, 2008

L.7. Kaplan* A, Lenner M, Huchon* C, Palmer* RE; Nonlinearity and time-resolved studies of ion emission in ultrafast laser ablation of graphite; *Appl Phys A;* **92**, 999-1004, 2008

L.8. Sidorov-Biryukov* DA, Fernandez* A, Zhu* L, Verhoef* A, Dombi P, Pugzlys* A, Serebryannikov* EE, Zheltikov* AM, Knight* JC, Baltuska* A; Solitonic dynamics of ultrashort pulses in a highly nonlinear photonic-crystal fiber visualized by spectral interferometry; *Opt Lett;* **33**, 446-448, 2008

L.9. Kroó N, Varró S, Farkas Gy, Dombi P, Oszetzky D, Nagy A, Czitrovszky A; Nonlinear plasmonics; *J Mod Opt*; accepted for publication

L.10. Kroó N, Farkas Gy, Dombi P, Varró S; Nonlinear processes induced by the enhanced, evanescent field of surface plasmons excited by femtosecond laser pulses; *Opt Express;* accepted for publication

Article in Hungarian

L.11. Farkas Gy; Attoszekundumos időtartamú fényimpulzusok és elektronimpulzusok (Attosecond-duration light pulses and electron pulses, in Hungarian), *Informatika* **10**, 33-43, 2008

See also: N.8.

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 performed extensive numerical simulations aiming to explore the shear viscosity of three-dimensional Yukawa liquids, which are frequently used as a model system of complex plasmas. The results obtained using two independent non-equilibrium simulation methods have been critically compared with each other and with earlier published data for a wide range of plasma coupling (Γ) and screening (κ) parameters. The non-Newtonian behavior of the liquid, manifested as a decrease of the shear viscosity with increasing shear rate (shear thinning), and the validity of the Stokes-Einstein relation at high coupling strengths have also been demonstrated. Detailed molecular-dynamics studies revealed the nature of high harmonic generation in a wide variety of 3D and layered many-particle systems due to the presence of non-linear wave-wave interactions. The emergence and vanishing of superdiffusion in quasi-two-dimensional Yukawa systems has been investigated by molecular dynamics simulations via the analysis of the asymptotic behavior of the mean-squared displacement of the particles and the long-time tail of the velocity autocorrelation function. We calculated the full density response function and from it the long-wavelength acoustic dispersion for a two-dimensional system of strongly coupled point dipoles interacting through a $1/r^3$ potential at arbitrary degeneracy. We have constructed an experimental system (the first in Hungary) for studies of dusty plasmas, which allows investigation of collective phenomena in strongly-interacting many-particle systems on the mesoscopic scale, in the theoretically hardly accessible strongly coupled domain. Our preliminary results show satisfying agreement between the experimental and computed wave dispersion properties of the dust-plasma crystal. Using the "Particle in Cell" simulation method we have analyzed properties of capacitively excited low-pressure gas discharges, with special attention to the sign reversals of the electric field and the associated heating of the electrons in the discharge. We have investigated possible improvements of the hybrid modeling techniques applicable for the description of low-pressure gas discharges and have been working on the development of a comprehensive modeling network for the description of analytical glow discharge cells.

Studies of post-discharge systems used for plasma sterilization. — The bactericidal effect of the Ar, Ar-O_2 and N_2-O_2 plasmas it is well known from the numerous experimental investigations carried out in many laboratories. In these plasmas the bactericidal role is played by the active atoms as N and O, and UV photons emitted by the excited atoms or molecules. With the aim to contribute to the optimization of the plasma based sterilization systems, and to the understanding of the role of different species in the sterilization process, we have developed discharge kinetic and post-discharge hydrodynamic models, which allow the study of post-discharge systems. Presently the afterglows of the flowing Ar, Ar-O_2 and N_2-O_2 microwave discharges are mostly used in the sterilization experiments. For these systems we have carried out detailed calculations at different discharge conditions, determining the species densities distributions in a large post-discharge reactor, where the tools to be sterilized can be placed. Our calculations have shown that in order to have a homogeneous density distribution in the reactor, providing the same bactericidal efficiency everywhere, low pressures, as 2 Torr and high gas flows, as 1000 sccm need to be used. With the model we could also determine the origin of the VUV/UV radiation in the different systems.

Electrolyte cathode atmospheric pressure glow discharge (ELCAD). – The ELCAD cell was fitted in an atomic absorption spectrometer (AAS3, Zeiss, Jena) and the decadic extinction $\lg(I_0/I)$ (which is proportional to the density of metal atoms) of Zn, Cd, Cu, Ca, Na, Pb and Cr were measured as a function of the distance from the cathode. The obtained extinctions showed a significant element dependency, similarly to that observed in the case of the emitted intensities. This latter was explained by the element dependency of the bond strength of M^+-OH^- complexes leaving the cathode due to the cathode sputtering. The measured decadic extinctions, in this way the density of metal atoms decreased with the distance from the cathode. This behavior is in accordance with the emitted intensity distributions. In the cases of the Cr-I 357-360 nm and 425-429 nm resonant lines, the measured values of $\lg(I_0/I)$ were about one order of magnitude lower compared with that received for other metal atoms. But, the emitted intensity of the Cr-I 520.4, 520.6 and 520.8 nm non-resonant atomic lines were observed to be one order of magnitude higher than that of the resonant lines mentioned above. Since the upper level energy of Cr-I 520.4-8 nm E_{up}=3.32 eV are between the E_{up}=2.9 eV of Cr-I 427nm and the E_{up}=3.45 eV of Cr-I 360 nm, the observed high intensity of the Cr-I 520 nm can be attributed to a selective excitation process and not to a direct electron impact one. Using the Cr-I 520.6 nm lines, the preliminary FIA (Flow Injection Analysis) experiments shows that the LOD value (Limit of Detection) for Cr is about 5 μg/ml, which can be decreased further by an improvement of the measuring system.

Multispectral imaging reflectometer. — The development of a new type of optical reflectometers was successfully finished, in cooperation with the Research Institute for Technical Physics and Materials Science, supported by a GVOP grant. The „pre-industrial" application of the prototype starts in Germany at the end of this year.

E-Mail:

Károly Rózsa	karcsi@sunserv.kfki.hu
Gergely Bánó	bano@sunserv.kfki.hu
László Csillag	csillag@szfki.hu
Aranka Derzsi	derzsi@sunserv.kfki.hu
Zoltán Donkó	donko@sunserv.kfki.hu
Péter Hartmann	hartmann@sunserv.kfki.hu
Péter Horváth	phorvath@sunserv.kfki.hu
Zoltán Gy. Horváth	horvath@szfki.hu
Igor Korolov	korigal@mail.kfki.hu
Kinga Kutasi	kutasi@sunserv.kfki.hu
Pál Mezei	mezeipal@szfki.hu

Grants and international cooperations

OTKA T-48389	Modern plasma simulation techniques (Z. Donkó, 2005–2008)
OTKA IN-69892	Simulation of strongly-coupled many-particle systems (Z. Donkó, 2006–2008)
MRTN-CT-2006-035459	GLADNET: Analytical Glow Discharge Network (Z. Donkó, 2007-2011)
OTKA PD-049991	Post-doc position (P. Hartmann, 2005–2008)
MTA-NSF/102	Advanced numerical modeling of strongly coupled many-particle systems (Z. Donkó, 2008-2010)
TÉT Port 14/2005	Electron kinetics in gas mixtures (Z. Donkó, 2006-2008)

MTA-CSIC #8	Use of kinetic methods to study the electron energy distribution function and plasma chemistry of SPRITE discharges produced in the mesosphere and lower ionosphere: Impact on the ozone chemistry. (Z. Donkó, 2007-2008)
OTKA-F-67556	Modelling of post-discharges used for sterilization and surface treatment (K. Kutasi, 2008 – 2010)
OTKA K-68390	Investigations of the atomization processes in the electrolyte cathode atmospheric glow discharge (P. Mezei, 2007-2011)

Publications

Articles

M.1. Donkó Z, Hartmann P; Shear viscosity of strongly coupled Yukawa liquids; *Phys Rev E*; **78**, 026408/1-8, 2008

M.2. Ott T* , Bonitz M* , Donkó Z, Hartmann P; Superdiffusion in quasi-two-dimensional Yukawa liquids; *Phys Rev E*; **78**, 026409/1-6, 2008

M.3. Donkó Z, Kalman* GJ, Hartmann P; Collective excitations and dynamical correlations of Yukawa liquids; *J Phys Cond Matter*; **20**, 413101/1-35, 2008

M.4. Golden* K I, Kalman* GJ, Donkó Z, Hartmann P; Acoustic dispersion in a two-dimensional dipole system; *Phys Rev B*; **78**, 045304/1-11, 2008

M.5. Schulze* J, Donkó Z, Heil* BG, Luggenhölscher* D, Mussenbrock* T, Brinkmann* RP, Czarnetzki* U; Electric field reversals in the sheath region of capacitively coupled radio frequency discharges at different pressures; *J Phys D: Appl Phys*; **41**, 105214/1-15, 2008

M.6. Feldmann* JD, Kalman* GJ, Hartmann P, Rosenberg* M; Ground state of magnetic dipoles on a two-dimensional lattice: structural phases in complex plasmas; *Phys Rev Lett*; **100**, 085001/1-4, 2008

M.7. Kutasi K, Saoudi* B, Pintassilgo* CD, Loureiro* J, Moisan* M; Modelling the low-pressure N_2-O_2 plasma afterglow to determine the kinetic mechanisms controlling the UV emission intensity and its spatial distribution for achieving an efficient sterilization process; *Plasma Processes and Polymers*; **5**, 840, 2008

M.8. Ajtony* Zs, Szoboszlai* N, Suskó* EK, Mezei P, György* K, Bencs L; Direct sample introduction of wines in graphite furnace atomic absorption spectrometry for the simultaneous of arsenic, cadmium, copper and lead content; *Talanta;* **76,** 627-634 , 2008

M.9. Guerra* V, Kutasi K, Lino* da Silva M, Sá* PA, Loureiro* J; Kinetic simulation of discharges and afterglows in molecular gases; *High Temperature Material Processes*; accepted for publication

M.10. Donkó Z; Molecular dynamics simulations of strongly coupled plasmas; *J Phys A: Math Theor*; accepted for publication

M.11. Donkó Z, Schulze* J, Heil* B G, Czarnetzki* U; PIC simulations of the separate control of ion flux and energy in CCRF discharges via the electrical asymmetry effect; *J Phys D: Appl Phys*; accepted for publication

Conference proceedings

M.12. Donkó Z, Hartmann P; On the shear viscosity of 3D Yukawa liquids; In: *Multifacetes of Dusty Plasmas (Proc. of 5th International Conference on the Physics of Dusty Plasmas, 18-23 May, 2008)*; Ed.: Mendonca JT, Resendes DP, Shukla PK, Ponta Delgada, Azores, Portugal; pp. 197-198, 2008

M.13. Hartmann P, Donkó Z, Kalman* GJ; Numerical studies of the melting transition in 2D Yukawa systems; In: *Multifacetes of Dusty Plasmas (Proc. of 5th International Conference on the Physics of Dusty Plasmas, 18-23 May, 2008)*; Ed.: Mendonca JT, Resendes DP, Shukla PK, Ponta Delgada, Azores, Portugal; pp. 219-220, 2008

M.14. Derzsi A, Hartmann P, Donkó Z; Improved fluid and hybrid modeling of low-pressure discharges by incorporating electron energy balance equation; In: *Proc.19th Europhysics Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG), 15-19 July 2008, Granada, Spain*; pp. 2-12, 2008

M.15. Derzsi A, Donkó Z, Bogaerts* A, Hoffmann* V; The influence of the secondary electron emission coefficient and the effect of the gas heating on the calculated electrical characteristics of a Grimm type glow discharge cell; In: *Proc. of 24rd Summer School and International Symposium on the Physics of Ionized Gases (SPIG), Novi Sad, Serbia, August 25 - 29, 2008*; Eds.: G.Malovic, L. Popovic, M.Dimitrijevic; pp. 285-288, 2008

M.16. Kutasi K, Saoudi* B, Pintassilgo* CD, Loureiro* J, Moisan* M; UV radiation distribution in N_2-O_2 post-discharges used for sterilization; In: *Proc.19th Europhysics Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG), 15-19 July 2008, Granada, Spain*; pp. 3-81, 2008

M.17. Kutasi K, Guerra* V, Sá* PA, Loureiro* J; Active species in Ar-O_2 microwave flowing post-discharges; In: *Proc. 19th Europhysics Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG), 15-19 July 2008, Granada, Spain*; pp. 2-42, 2008

M.18. Kutasi K, Guerra* V, Sá* PA, Loureiro* J; Modeling of a flowing Ar-O_2 microwave discharge and post-discharge; In: *Proc. of 24rd Summer School and International Symposium on the Physics of Ionized Gases (SPIG), Novi Sad, Serbia, August 25 - 29, 2008*; Eds.: G.Malovic, L. Popovic, M.Dimitrijevic; pp. 351-354, 2008

Conference proceeding in Hungarian

M.19. Mezei P, Cserfalvi* T, Bencs L, György K; Elektrolitkatódos atmoszférikus kisülés vizsgálata atomabszorpciós spektroszkópiával (Investigations of an electrolyte cathode atmospheric discharge by atomic absorption spectroscopy, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; P-32, 2008

Patent

M.20. Horváth ZGy, Juhász* G, Fried* M, Major* C, Petrik* P; Pinhole kamerát alkalmazó leképző optikai vizsgáló berendezés (Imaging optical testing devise using a pinhole camera); P0700366

N. LASER APPLICATION

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

Extreme light infrastructure development. — One of the main activities of our department is the participation in EU FP7 Extreme Light Infrastructure (ELI) –ESFRI Project in which 13 countries are involved. ELI would be the first infrastructure dedicated to the fundamental study of laser-matter interaction in a new and unsurpassed regime of laser intensity: the ultra-relativistic regime ($I_L>10^{23}$ W/cm²). At its centre would be an exawatt-class laser ~1000 times more powerful than either the Laser Mégajoule in France or the National Ignition Facility (NIF) in the US. In contrast to these projects, ELI would attain its extreme power from the shortness of its light pulses (femtosecond and attosecond). This will give us the possibility to study ultrafast processes from molecules to quarks at the attosecond timescale. A recent revolution in laser technology has opened the door to a 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 power densities exceeding $I_L>10^{25}$ 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 afford 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. Beside the leading of WP 4, in this project we are participating in almost all Work Packages. At different WP meetings (the WP4 meeting was organised in Budapest) we clarified our participation in the scientific and technical programs at the next step of the project. Our responsibility will be the interferometric testing of optical surfaces with nanometer resolution, development and production of special optical coatings (AR, beam splitters, mirrors, etc.), development of special metrologic equipment to measure statistical parameters, participation in building of certain optical parts. A proposal for Hosting ELI facility in Hungary was also applied. For this application we elaborated the needed technical and other documentation, prepared a lot of presentations and organised a dozen of meetings and discussions.

Optical measuring techniques. — In this year we developed a portable industrial version of the dual wavelength optical particle analyzer enabling simultaneous measurement of the concentration, size distribution, refractive index and absorption of aerosol particles. This instrument is controlled by a laptop PC, but has also a built-in control panel, where the actual status and the main parameters are displayed.

Fig. 1. The portable version of the dual wavelength optical particle analyzer

[#] Ph.D. student

After appropriate calibration performed using a TSI Small-Scale Powder Disperser (SSPD), different kind of aerosol generators, and a Differential Mobility Analyzer, we tested the device at different conditions and improved the software enabling the display of measured parameters in 2D and 3D diagrams.

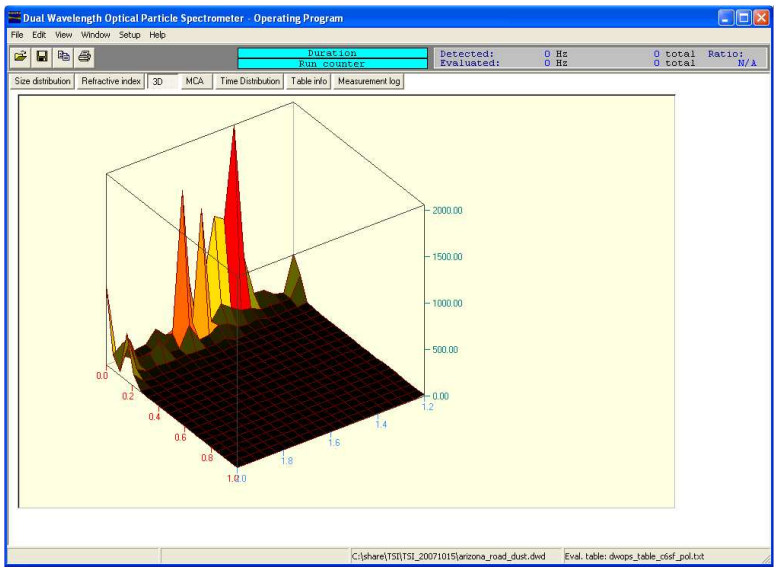


Fig. 2. The distribution of the complex refractive index of aerosol particles

The measured parameters can help us to determine the origin of the aerosol contamination and give more complete information about the particles as any existing device in this field. The other benefit of the developed device is the possibility to perform 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.

Using the newly developed airborne particle counter installed in our mobile laboratory (van) several measurement campaigns were organised where we measured the atmospheric aerosols and toxic gases in different location during different seasons of the year. During the measurement campaigns performed using the mobile laboratory air contamination maps in Budapest airport and its surrounding were composed. The collected data were compared with the statistics of the adverse health effects to the pregnancy where significant negative influence was determined. The aerosol particle deposition in human airways was modelled and specific deposition parameters were determined in case of diseased airways.

In the frame of this project the time resolution of single photon detectors were measured with a new setup proposed. The measurements were carried out for some commercially available avalanche photodiodes and modules. It was established that the time resolution (FWHM) is in the range of 30 ps. The time resolution is the key parameter in the proposed measurement system. A multi channel timing analyzer & multi channel amplitude analyzer module (MCTA – MCAA) system card was designed and constructed and implemented as a PXI module. The measurement system using DSP technology was constructed and is currently under electronic and field tests.

Model studies were carried out for the accuracy of number concentration measurement depending on the wavelength and refractive index of measured particles.

In the frame of common project with the Technical University of Budapest a Digital Holographic System (DIADEM +) was developed. The laboratory version of this system was finalized and tested using different model samples.

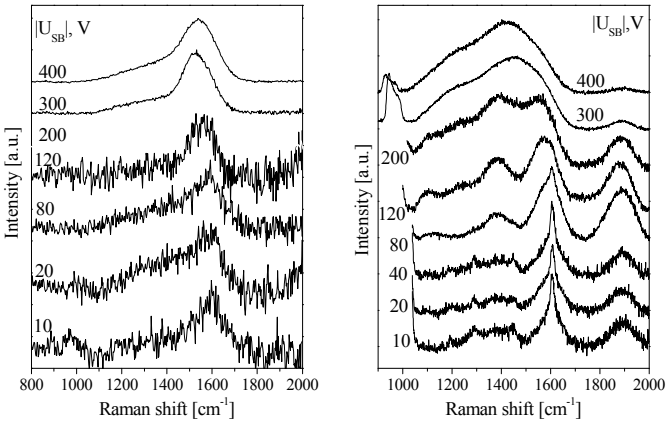
Measurement of the statistics of photons generated in different nonlinear optical processes were performed. The surface plasmon generation and their statistical properties were studied. The statistics of the excitation light and the light generated by surface plasmons was compared. The temporal statistical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

A new size estimator algorithm was developed for the simultaneous measurement of nanoparticle velocity and size in photon counting, photon correlation experiments. The model system uses a laser Doppler anemometer (LDA) fringe pattern measurement volume. The model was extended for some exotic particle composition and shape e.g. spherical particles with inclusions, cylindrical particles, coated particles, etc. It was established that the practical limits in size range are 50 – 500 nm for particles in the moderate refractive index range. Accurate single particle sizing is available at low photon rates such as 50 counts per burst. Smaller detection limits are applicable for special metallic particles. The model makes use of standard techniques of Lie filtering, burst selecting and model based optimization algorithm with the auto-correlation function as the figure-of-merit. The limits of applicability of this method for the on-line, in-situ single particle velocity and size detection and particle number concentration were established. Preliminary experiments were carried out for checking the model. On the encouragement of industrial partners a grant was obtained for the financing of the development of a commercial device.

Amorphous carbon layers. — Spectroscopic methods were used to characterize atomic bonding properties and electronic levels localized near band edges of different carbon-based materials. Amorphous, nano-, and ultra-nanocrystalline (NCD, UNCD) carbon-based films are promising materials of modern technology due to their unique and advantageous mechanical, electrochemical, electronic and optical properties. In amorphous carbons, the sp^3 phase and H incorporation define the skeletal matrix which controls the mechanical properties, while the sp^2 phase content and organization controls the density of states deep in the gap and, therefore, the optical gap and the electronic properties. The presence of both sp^2 and sp^3 phases diversifies the range of possible electronic and structural modifications. Nano-crystalline diamond thin films have composite structure where the diamond crystallites are embedded into an amorphous carbon matrix. Beside the average grain size, the properties of grain boundaries are the most important factors affecting the film properties.

Raman spectroscopy is widely used for the characterization of these materials. The whole interpretation and evaluation of the Raman spectra on amorphous carbon is based on the decomposition of the curve in the 1000-1650 cm^{-1} region into two components – the G and D peaks. However the use of two peaks for the decomposition of the Raman spectra of a-C:H thin films is inaccurate, so as the fitted curve differs from the experimental one. This suggests that not only structural units, vibrating at frequencies of G and D peaks, contribute to the spectra. However, since it is difficult to determine the parameters of the extra peaks, the attempts made for their assignment lead to controversial results. One way to obtain more precise information on these bands is to change excitation wavelength, since the dispersion of the peaks is different, then the overlapping peaks can separate.

We have shown that the near-infrared excited Raman scattering can serve additional information on the structure of different a-C:H films compared to the visible excitation. Our results obtained on a-C:H thin films prepared from benzene demonstrate that the Raman spectrum of amorphous carbon in the 1000 – 1700 cm^{-1} region consists of four bands and that these bands can be assigned to vibrations of definite structural units. For comparison, Raman spectra obtained by 488 nm and 785 nm probe wavelengths are shown in Fig.3 for a-C:H samples prepared from benzene at different self-biases. The self-bias dependence of component bands determined by the deconvolution of Raman spectra measured by 785 nm probe wavelength can be seen in Fig.4. We have pointed out that the G band consists of two peaks one of which have been assigned to C–C stretching vibration of long chain clusters composed by sp^2 carbon atoms, while the other one arises from C–C stretching vibrations of small-sized aromatic sp^2 clusters. Hence we proved that not only the aromatic rings contribute exclusively to scattered light in the G band region as it was thought earlier.



(a) (b)

Fig.3. *488 nm (a) and 785 nm (b) excited Raman spectra of a-C:H thin films prepared form benzene at different self-bias voltages.*

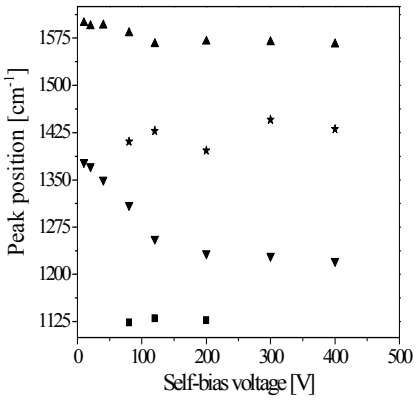


Fig.4. *Dependence of the peak positions observed in 785 nm excited Raman spectra of a-C:H thin films prepared form benzene at different self-bias voltages.*

Analysis of the 785 nm excited Raman spectra measured in different points of nanocrystalline diamond thin films using small excitation volume indicated that there are some changes appear in the spectra when moving the excitation spot to another place on the surface. For the detailed analysis of the above mentioned phenomenon a series of spectra were measured along a 25 μm long line with 0.5 μm steps with both 785 nm and 488 nm excitations. The excitation spot diameter was set to 1 μm in both cases. Raman spectra measured in different points are shown in Fig.5. The 488 nm excited spectra taken in different points are very similar and they reveal the well known UNCD Raman spectrum with its characteristic peaks together with second-order Raman peak of the Si substrate appearing around 960 cm^{-1}. From these data one can conclude that this film is of homogeneous structure and it is built up of relatively large diamond crystallites. In contrary, the analysis of he 785 nm excited spectra recorded in the same points as the 488 nm excited ones leads to just the opposite conclusions regarding the homogeneity and structure of the NCD film. The huge differences in the character of the upper three spectra in Fig. 5 suggest that the structure of the diamond film in the measurement points differ significantly. The narrow peaks have high intensity but only a few of them present in each spectrum in Fig.5. To obtain general information on the most frequent peaks, series of spectra were measured and the results of statistical analysis can be seen in Fig.6. It is

interesting to note that the 1334 cm^{-1} diamond peak is not the most frequent one, which shows that there are spectra measured on the NCD sample lacking this peak at all. The assignment of some narrow peaks we have published earlier. Recent results prove that the broad bands in the NCD spectra are composite ones and their components can be enhanced selectively. The lateral scan of the sample with 0.5 μm steps and excitation spot of 1 μm diameter proves that the Raman scattering with 785 nm excitation is highly sensitive to smallest differences in the structure and it allows the detection and determination of the Raman peaks arising from the definite regions of the sample.

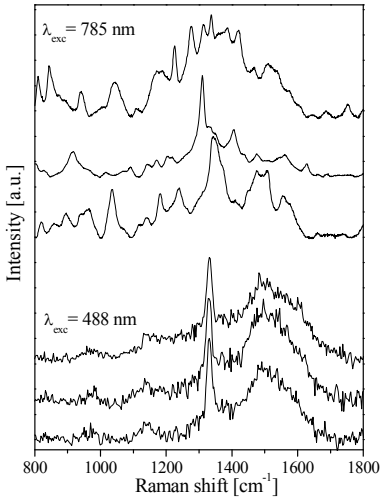


Fig.5. *Comparison of Raman spectra of nanocrystalline diamond film measured in different points of the sample surface using 785 nm and 488 nm excitation wavelengths.*

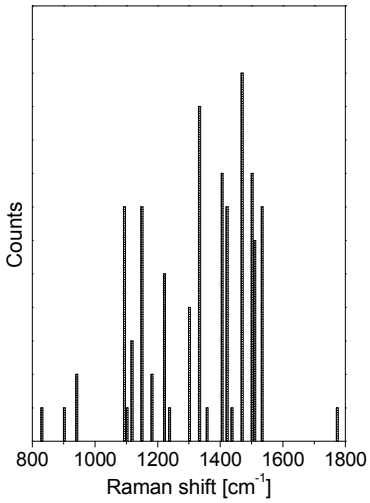


Fig. 6. *Most frequent Raman peaks in a set of 50 spectra taken along a 25 μm line on the NCD surface with steps of 0.5 μm.*

Carbon based thin film coating of porous material surface is of practical importance. Electronic levels localized near band edges of carbon nanostructure deposited onto the oxidized Al and Ta surface we have monitored by photoluminescence measurements. The carbon films on both porous substrates are of large band gap material with intensive blue light emission at room temperature. The distribution of tail states is broadened for carbon film on the oxidized Al substrate compared to film deposited onto oxidized Ta surface. These properties correlate with atomic bonding properties of carbon films determined from Raman measurements.

E-Mail:

Aladár Czitrovszky	czi@szfki.hu, czitrovszky@sunserv.kfki.hu
Péter Jani	pjani@sunserv.kfki.hu
Árpád Kiss	kissa@szfki.hu
Margit Koós	koos@szfki.hu
Attila Nagy	anagy@szfki.hu
Dániel Oszetzky	odani@szfki.hu
Sára Tóth	tothsara@szfki.hu
Lénárd Vámos	vamos@szfki.hu
Miklós Veres	vm@szfki.hu

Grants and international cooperations

NKFP-3A/089 National Research and Development Program, Environmental Pollution of the Atmosphere (Coordinator: A. Czitrovszky, 2004-2008)

OTKA T-043359 Preparation and complex characterization of carbon based nanocomposites (M. Koós, 2005-2008)

GVOP-3.1.1. No 0403/3.0, DIADEM (in cooperation with Budapest Technical University) (A. Czitrovszky, 2005-2008)

108/C HAS Development of Aerosol Analyzer (Coordinator A. Czitrovszky, 2007-2008)

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 (Coordinator A. Czitrovszky, 2007-2010, 0217/2007 SZFKI-MTA HAS Support for the grant No 0217/2007/OM)

212105/ELI EU FP7 ESFRI, Extreme Light Infrastructure, Coordination of Hungarian participants (Coordinator: A. Czitrovszky, 2007-2010)

410/EAC EAC Conference (Coordinator: A. Czitrovszky, 2008)

Bilateral Austro-Hungarian Cooperation, Contract No A-20/01 (A. Czitrovszky, 2005-2008)

Bilateral Hungarian-Ukrainen Cooperation: Laser annealing and monitoring structural transformation in holographic and optical media based on binary chalcogenide glasses during recording Raman spectra at different energies of excitation, Contract No. UA-2/2006 (M. Koós 2007-2008)

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

Publications

Articles

N.1. Veres M, Tóth S, Kukovecz* Á, Koós M; Spatially resolved near-infrared excited Raman spectroscopy of nanocrystalline diamond films; *Diamond and Related Materials*; **17**, 515-519, 2008

N.2. Veres M, Tóth S, Koós M; New aspects of Raman scattering in carbon-based amorphous materials; *Diamond and Related Materials*; **17**, 1692-1696, 2008

N.3. Kovács* Gy J, Veres M, Koós M, Radnóczi* G; Raman spectroscopic study of magnetron sputtered carbon–nickel and carbon nitride–nickel composite films: The effect of nickel on the atomic structure of the C/CNx matrix; *Thin Solid Films*; **516**, 7910-7915, 2008

N.4. Kovach* G, Karacs* A, Radnoczi* G, Csorbai* H, Guczi* L, Veres M, Koós M, Papadimitriou* L, Sólyom* A, Pető* G; Modified π-states in ion-irradiated carbon; *Applied Surface Science*; **254**, 2790-2796, 2008

N.5. Vámos L, Jani P; Lee filtered burst selecting in the photon correlation LDA signal processing; *SPIE Int Soc Opt. Eng*; 7003A-41, 1-8, 2008

N.6. Vámos L, Jani P; Nanoparticle sizing algorithm for photon correlation LDA; *Meas Sci Technol*; accepted for publication,

N.7. Szymanski* WW, Nagy A, Czitrovszky A; Optical particle spectrometry problems and perspectives; *Journal of Quantitative Spectroscopy and Radiative Transfer*; accepted for publication

N.8. Oszetzky D, Kroó N, Nagy A, Czitrovszky A; Study of surface plasmon statistics by optical methods; *SPIE Proceedings*; accepted for publication

Conference proceedings

N.9. Czitrovszky A, Oszetzky D, Nagy A; Experimental realization of pre-programmed photon source and other applications of entangled states; In: *Int. Conference of Advanced Laser Technologies, Sept. 13-18, Siófok, Hungary*; pp. 119-120, 2008.

N.10. Nagy A, Czitrovszky A, Szymanski* W; Calibration and experimental evaluation of the Dual Wavelength Optical Particle Spectrometer; In: *Proc. European Aerosol Conference, Aug. 25-29, Thessaloniki, Greece*; pp. 66-67, 2008.

N.11. Nagy A., Czitrovszky A, Szymanski* WW; Calibration and experimental evaluation of the Dual Wavelength Optical Particle Spectrometer, In: *Proc. European Aerosol Conference, Aug. 25-29, Thessaloniki, Greece; 2008*.

N.12. Szymanski* WW, Nagy A, Czitrovszky A; Optical particle spectrometry problems and perspectives; In: Proc. *Ges. Für Aerosol Forschung Meeting, 1-3 July, 2008, Karlsruhe, Germany*

Conference proceedings in Hungarian

N.13. Oszetzky D, Nagy A, Czitrovszky A; Programozható fotonszámú fényforrás (Programmable photon source, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; pp. 34-35, 2008.

N.14. Czitrovszky A, Osvay* K, Szabó* G, Sánta* I, Földes* I; Magyar részvétel az ELI programban (Hungarian participation in ELI project, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; pp. 4-5, 2008.

N.15. Füzessy* Z, Gyimesi* F, Czitrovszky A, Molnárka* Gy, Szigethy* D; Megnövelt felbontású és látóterű digitális holográfia (Digital holography with enhanced resolution and view field, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; pp. 5-6, 2008.

Book chapters

N.16. Veres M, Tóth S, Perevedentseva* E, Karmenyan* A, Koós M; Raman spectroscopy of UNCD grain boundaries; NATO Science Series, Springer Science, accepted for publication

N.17. Mitsa* V, Holomb* R., Veres M., Koós M.; Raman szórás nanoszerkezetű kalkogenid üvegekben (Raman scattering of nannostructured chalcogenide glasses); *Ungvári Nemzeti Egyetem*, accepted for publication

See also L.9.

O. FEMTOSECOND LASERS

R. Szipőcs, J. Fekete, P. Antal

Continuing our research on one- and two-dimensional photonic bandgap (PBG) structures, i.e. multilayer dielectric mirrors and photonic crystal fibers (PCF-s), we proposed that one-dimensional dielectric structures should be used at grazing incidence of light in order to obtain an extended bandgap exhibiting considerably reduced reflection loss and dispersion compared to similar structures used at normal incidence of light. The well-known quarter-wave condition was applied for the design in this specific case, resulting in resonance-free reflection bands without drops in reflection versus wavelength function and a monotonous variation of the group delay dispersion (GDD) versus wavelength function, which are important issues in femtosecond pulse laser applications. Based on these results we extended our studies to two-dimensional PBG structures and provided guidelines to the design of leaking mode-free hollow-core Bragg PBG fibers providing anomalous dispersion over most of the bandgap.

In hollow core photonic crystal fibers, most of the optical power is guided in the air core, which allows delivery of femtosecond laser pulses with energies in the 1 to 10 nJ regime without considerable nonlinear distortion. This feature makes them attractive for applications that require single mode delivery of relatively large energy ultrashort pulses, such as miniaturized multiphoton microscopes. The dispersion profile of state of the art photonic bandgap fibers, however, has the “canonical form” for bandgap guidance, which is basically a third-order function monotonically increasing from short to longer wavelengths. For most applications, such as time resolved spectroscopy, nonlinear optics including nonlinear microscopy, etc., however, nearly transform limited, high quality optical pulses are preferred.

In collaboration with researchers at Furukawa Electric Institute of Technology Ltd. and R&D Ultrafast Lasers Ltd., 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. The canonical form of the dispersion profile in photonic bandgap fibers was modified by a partial reflector layer/interface placed around the core forming a 2D cylindrical Gires-Tournois type interferometer. This small perturbation in the index profile induces a frequency dependent electric field distribution of the preferred propagating higher-order-mode resulting in a zero or reversed dispersion slope (see Fig.1).

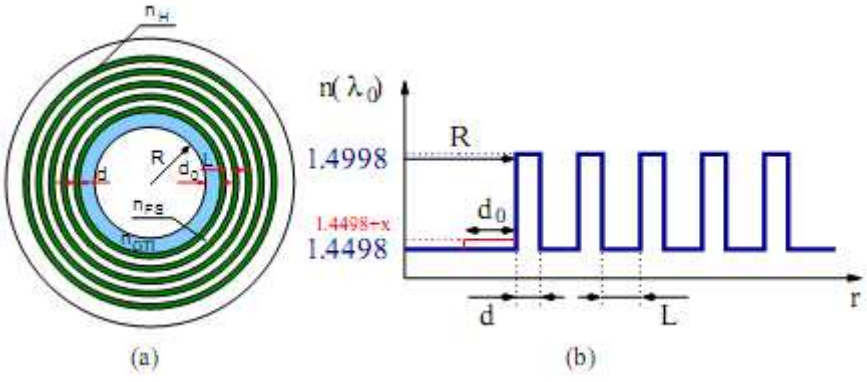


Fig. 1 *(a) SC Bragg PBG fiber used for finite-element calculations, (b) 1D equivalent of a SC Bragg PBG fiber.*

In collaboration with researchers at Furukawa Electric Institute of Technology Ltd. and R&D Ultrafast Lasers Ltd., an all-fiber, all-normal dispersion ytterbium ring laser was developed. It produces stable mode-locking of ~10 ps pulses that can be externally compressed to as short as ~200 fs. The experimental setup is shown in Fig. 2. In collaboration with the R&D Ultrafast Lasers Ltd. the output of this oscillator was amplified by a two-stage amplifier chain resulting in averaged mode-locked output power as high as 660 mW with compressed pulse duration of ~300 fs.

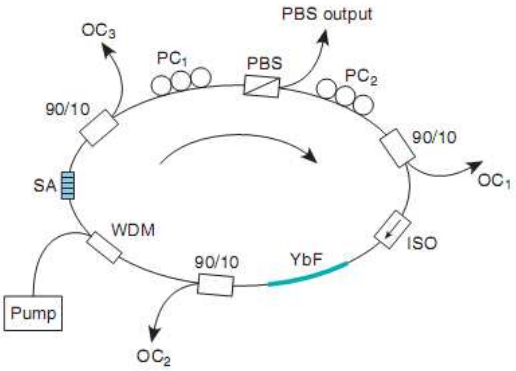


Fig. 2. *Experimental setup of the Yb fiber laser (PBS: polarizing beam splitter; PC: polarization controller; 90/10: 90/10 splitter; OC: output coupler; ISO: isolator;YbF: Yb-doped fiber; WDM: wavelength division multiplexer; SA: saturable absorber)*

Saturable absorber mirrors play an important role in mode-locking of bulk solid state or fiber based femtosecond oscillators (see above). In collaboration with Biological Research Center Szeged of HAS and R&D Ultrafast Lasers Ltd, a pump-probe time resolved spectroscopic system was developed, which was successfully applied for measurement of the transient absorption response of semiconductor based saturable absorber mirrors (SESAM). A typical measured transient absorption function of SESAM used for mode-locking a Ti:sapphire laser is shown in Fig.3.

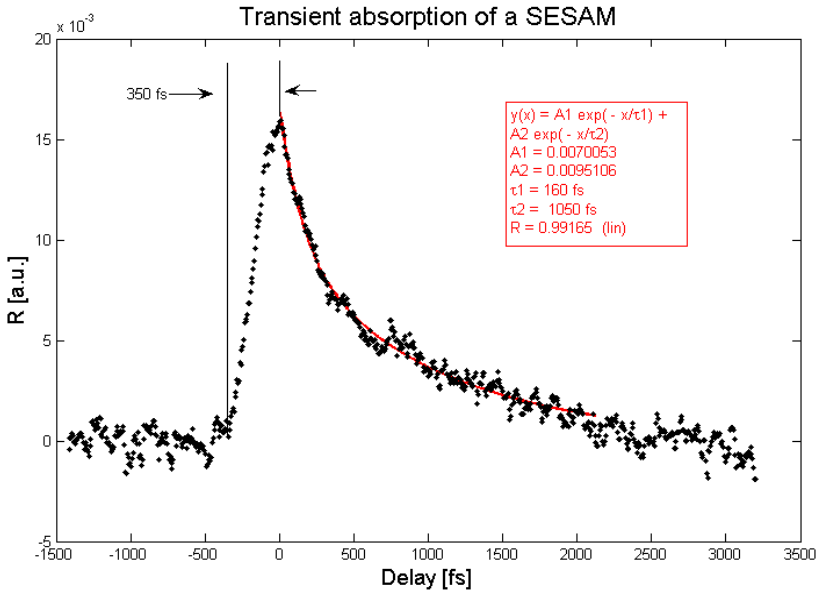


Fig. 3. Measured transient absorption function of a SESAM.

E-Mail:

Péter Antal	antal@szfki.hu
Júlia Fekete	feketej@sunserv.kfki.hu
Róbert Szipőcs	szipoecs@sunserv.kfki.hu

Grants and international cooperations

OTKA T-049296 Propagation of ultrashort laser pulses in photonic crystal fibers and fiber amplifiers (R. Szipőcs, 2005-2008)

OTKA T-048725 Ultrafast linear and nonlinear processes in macromolecules (R. Szipőcs, 2005-2008)

NKFP1-00007/2005 National Research and Development Program – Femtobiology (Coordinator: R. Szipőcs, 2006-2008)

Contract

SZFKI-R&D Ultrafast Lasers Ltd: Research and development of femtosecond pulse pump-probe spectroscopic system (Coordinator: R. Szipőcs, 2006-2008)

Publications

Articles

O.1. Várallyay* Z, Saitoh* K, Fekete J, Kakihara* K, Koshiba* M, Szipőcs R; Reversed dispersion slope photonic bandgap fibers for broadband dispersion control in femtosecond fiber lasers; *Optics Express;* **16**, 15603-15616, 2008

O.2. Fekete J, Várallyay* Z, Szipőcs R; Design of high bandwidth one- and two-dimensional photonic bandgap dielectric structures at grazing incidence of light; *Appl Optics*; **47**, 5330-5336, 2008

O.3. Fekete J, Cserteg* A, Szipőcs R; All-fiber, all-normal dispersion ytterbium ring oscillator; *Laser Physics Letters;* **6**, 49-53, 2009

Conference proceedings

O.4 Fekete J, Várallyay Z* , Szipőcs R; Design of leaking mode free hollow-core photonic bandgap fibers; In: *Optical Fiber Communication Conference*; OSA Technical Digest Series (Optical Society of America, 2008), paper JWA4 , 2008

O.5 Várallyay Z* , Fekete J, Szipőcs R; Higher-order mode photonic bandgap fibers with reversed dispersion slope, In: *Optical Fiber Communication Conference*; OSA Technical Digest Series (Optical Society of America, 2008), paper JWA8 , 2008

O.6. Várallyay Z* , Fekete J, Szipőcs R; Higher order mode photonic bandgap fibers for dispersion control; In: *Conference of Lasers and Electro-Optics*; OSA Technical Digest Series (Optical Society of America, 2008), paper JThA48, 2008

Conference proceedings in Hungarian

O.7. Várallyay* Z, Fekete J, Szipőcs R; Fotonikus kristály szerkezetű optikai szál fordított diszperziós karakterisztikával (Inverted dispersion slope photonic crystal

fiber); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; P-37, 2008

O.8 Antal P, Szipőcs R; Hangolható, femtoszekundumos, hosszúrezonátoros Ti-zafír lézer (Tunable, long-cavity femtosecond pulse Ti:sapphire laser); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; P-17, 2008

O.9 Fekete J, Cserteg* A, Szipőcs R; Módusszinkronizált, normál diszperziójú szálintegrált itterbium ring oszcillátor (Mode-locked, all-fiber, all-normal dispersion ytterbium ring oscillator); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; P-24, 2008

O.10 Sándor* P, Makai* A, Szipőcs R; Szélessávú femtoszekundumos PPLN OPO időfelbontásos lézerspektroszkópiai vizsgálatokhoz (Broadband femtosecond pulse PPLN OPO for time resolved spectroscopic studies); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; P-35, 2008

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 refined our electron-beam deposition technology for producing of optical coatings containing nanooptically thin titania, silica, tantala, alumina, hafnia layers. Using the latest multiple target thin film optimisation method, we have developed high efficiency low dispersion thin film polarizer coatings for high-power femtosecond Ti:sapphire amplifiers, low dispersion wide-band antireflection coatings for periodically polarized $LiNbO_3$ crystals, low dispersion wide-band beamsplitter coatings for ultrafast applications in the IR range, for example. Our thin indium-tin-oxide (ITO) layers having electrical resistance in the kohm range were successfully applied on the top of optical waveguide sensor structures, because their optical absorptance is very low in the red part of the visible spectrum.

Superpolishing technology. – We have started new research project concerning the development of advanced optical polishing technologies for producing very smooth (lower than 0.4 nm rms surface roughness) optical glass and fused silica surfaces. We are using ceria based polishing formulas manufactured by nanotechnological methods for final polishing of our optical substrates made from BK7 type optical glass or Suprasil 1 type fused silica. The combination of "superpolishing" technology with ion-assisted deposition technology will open the door for producing very low loss and very stable laser mirror coatings on large size substrates too.

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

E-Mail:

Kárpát Ferencz optilab@t-online.hu

Contract

OPTILAB-SZFKI No. 2400/2008

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)

Publications

Articles

P.1. Hámori* A, Serényi* M, Dér* A, Ferencz K, Kökényesi* S; All-optical switching possibilities for optical packet switching; *Proceedings of the European Microwave Association*; **4**; pp. 221-225, 2008

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. — Pr-doped $YAl_3(BO_3)_4$ (YAB) single crystals were grown by the high temperature top seeded solution growth (HTTGS) method from $K_2O/MoO_3/B_2O_3$ flux. Pr^{3+}-transitions from the $^3H_4$ ground state to the $^3H_6$, $^3F_2$, $^3F_3$, $^3F_4$, $^1G_4$, $^1D_2$, $^3P_0$, $^3P_1$+$^1I_6$, and $^3P_2$ manifolds were detected and analyzed. Following the temperature dependence of the absorption lines, all the possible Stark components of these manifolds were identified, including the ground state sublevels. Some of the absorption lines split into components, that was attributed to slightly different lattice sites for Pr. After 458 nm excitation at room temperature ($^3P_2$ level) the dominant luminescence emission bands belonged to the $^1D_2 \rightarrow {}^3H_4$ transition around 16500 cm^{-1}. Weak emissions around 15500 cm^{-1} and 20400 cm^{-1} were attributed to $^3P_0 \rightarrow {}^3F_2$ and $^3P_0 \rightarrow {}^3H_4$ transitions, respectively. After 464 nm excitation at 8K $^3P_1 \rightarrow {}^3F_4$, $^3P_0 \rightarrow {}^3F_3$, $^1D_2 \rightarrow {}^3H_5$ and $^3P_1 \rightarrow {}^3F_3$ emissions were also identified.

Growth and study of lithium- and potassium/lithium-niobate single crystals with different compositions and doping. — Yb-doped (0.1-0.3 mol%) stoichiometric $LiNbO_3$ crystals were grown by HTTGS method from K_2O containing flux. The Li/Nb ratio (~0.998) in the crystals was determined from the UV absorption edge positions. The absorption and luminescence spectra of the Yb^{3+} ion were measured in the 8-300 K temperature range and compared to those of Yb and (Mg+Yb)-doped congruent crystals. The structure of the absorption and luminescence bands related to the Stark levels were similar in all these crystals, but significant narrowing of the lines was observed in the stoichiometric samples, especially in the 930-960 nm wavelength range. The splitting of the $^4F_{7/2}(1) \rightarrow {}^4F_{5/2}(2)$ band into at least six components was related to the non-equivalent local environments of Yb^{3+} ions. Accurate energy scheme of the Yb^{3+} ions in stoichiometric $LiNbO_3$ was established.

The periodically inversed domain structure in the ferroelectric $LiNbO_3$ crystal (PPLN) exhibits unique nonlinear optical properties applicable in integrated optics. PPLN crystals were grown by the off-centered Czochralski technique. Mg dopant above a threshold concentration inhibits the photorefractive laser damage but deteriorate the domain structure. Using Mg+Y and Zr+Y codopants resulted in better domain structure and proper laser resistance.

Growth and study of bismuth tellurite (Bi_2TeO_5) crystals. — Bi_2TeO_5:Yb,Tm double doped crystals were grown by the Czochralski technique. The absorption and luminescence properties of the crystal were determined. Energy transfer was discovered in both Tm→Yb and Yb→Tm directions. After excitation at 800 nm (Tm $^3H_4$-level), besides the Tm-emission, the $^2F_{5/2} \rightarrow {}^2F_{7/2}$ (Yb) emission was also detectable (Tm→Yb transfer). After excitation at 980 nm (Yb $^2F_{5/2}$-level) besides the Yb-emission, higher energy Tm-emissions ($^3H_4 \rightarrow {}^3H_6$, $^1G_4 \rightarrow {}^3H_6$) were identified (Yb→Tm transfer and up-conversion). The kinetics of the Tm-emission was followed by its intensity dependence upon the of 980 nm excitation. Accordingly, the $^3H_4 \rightarrow {}^3H_6$ emission corresponded to two-photon mechanism (log. slope: 1.82). The time dependence showed a slow build-up period after the pulsed excitation (400 μs) and a subsequent single exponential decay. The $^1G_4 \rightarrow {}^3H_6$ Tm-emission corresponded to three-photon mechanism (log. slope 3.08).

[#] Ph.D. student

Ho, Tm and Tb-doped Bi_2TeO_5 crystals were grown for memory substrate in volume holographic recording. Using continuous 532 nm Nd:YAG laser emission for writing, Ho and Tm act as both source and trap in the photorefractive process, Tb only as trap. Ho increased the photorefractive sensitivity of the host crystal (faster build-up of the signal), while the Tm increased the saturation diffraction efficiency. Using ns range write laser pulses, the undoped Bi_2TeO_5 exhibited the best performance. These dopants had no significant effect on the favorable self-fixing properties of the Bi_2TeO_5 crystal. The undoped crystals had the best optical properties, and this was dominant in the low bit error rate of the page oriented digital holograms.

Development of analytical methods for material science and environmental control. — In the frame of bilateral cooperation, mass, ionic composition of $PM_{2.5}$ (particle matter with aerodynamical diameter <2.5μm) aerosols and related gaseous pollutant were monitored in Northern Belgium at urban, suburban, industrial, and rural sampling sites. The diurnal average ratio of the ionic fraction was 40 % of $PM_{2.5}$, but sometimes it reached as high values as 80-98 %. The ionic fraction mostly consisted of SO_4^{2-}, NO_3^-, NH_4^+, and Na^+. The nitrogen and sulphur oxidization ratios demonstrated a low-to-moderate secondary aerosol formation over the region. Source apportionment showed vehicular emission, coal/wood burning, and animal farming as the dominating sources of ionic fraction in $PM_{2.5}$. These experimental data are comparable with the modeled values of the mass and ionic species in $PM_{2.5}$ acquired with the BelEUROS air-quality model.

NO_2 concentrations were monitored to evaluate the air quality before and after the infrastructural change of an important traffic artery in Mortsel, Antwerp (Belgium). The contribution of NO_2 was at the same level before and after the road works, i.e., it ranged from 30 to 73 $\mu g/m^3$ for the different sampling sites. The modernization work had no impact on preventing the traffic-related pollutant, NO_2 and as a consequence no significant effect on the air quality in the studied region.

The transport and deposition of suspended particulate matter (SPM) brought in by visitors was studied in the Royal Museum of Wawel Castle in Cracow, Poland. The deposited mass of SPM and the concentration of each element detected were considerably higher during the intensive tourist flow in summer, which was especially valid for soil-dust associated elements (Si, K, Ca, Al, and Ti).

A multi-element graphite furnace atomic absorption spectrometry (GFAAS) method was elaborated for the simultaneous determination of As, Cd, Cu, and Pb in wine samples of various sugar contents. For comparative GFAAS analyses, direct injection and digestion-based methods were optimized with the application of Pd-based chemical modifiers. The results obtained with these methods are in good agreement.

E-Mail

László Bencs	bencs@szfki.hu
Elena Beregi	beregi@szfki.hu
Gabriella Dravecz	dravecz@szfki.hu
István Földvári	foldvari@szfki.hu
Krisztina György	kriszta@szfki.hu
Ágnes Péter	apeter@szfki.hu
Katalin Polgár	polgar@szfki.hu
Zsuzsanna Szaller	szaller@szfki.hu

Grants and international cooperations

OTKA T-046481 Growth and spectroscopic investigation of self-frequency-doubling laser crystals (I. Földvári, 2004-2008)

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 of 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)

Publications:

Articles

Q.1. Samek* L, De Maeyer-Worobiec* A, Spolnik* Z, Bencs L, Kontozova* V, Bratasz L, Kozlowski* R, Van Grieken* R; Impact of electric overhead radiant heating on the indoor environment of historic churches; *J Cultur Heritage;* **8**, 361-369, 2007

Q.2. Péter Á, Hajdara I, Lengyel K, Dravecz G, Kovács L, Tóth* M; Characterization of Potassium Lithium Niobate (KLN) Ceramic System; *J Alloys & Comp*; **463**, 398-402, 2008

Q.3. Kontozova-Deutsch* V, Krata* A, Deutsch* F, Bencs L, Van Grieken* R; Efficient separation of acetate and formate by ion chromatography: Application to air samples in a cultural heritage environment; *Talanta;* **75**, 418-423, 2008

Q.4. Horn* W, Földvári I, Denz* C; Holographic data storage in photorefractive bismuth tellurite; *J Phys D: Appl. Phys;* **4**1, 224006/1-9, 2008

Q.5. Bencs L; Calculation of the spectral line profile broadening parameter in graphite furnace atomic absorption spectrometry; *Canadian J Anal Sci Spect;* **53**, 52-58. 2008

Q.6. Deutsch* F, Vankerkom* J, Janssen* L, Janssen* S, Bencs L, Van Grieken* R, Fierens* F, Dumont* G, Mensink* C; Modelling concentrations of airborne primary and secondary PM_{10} and $PM_{2.5}$ with the BelEUROS-model in Belgium; *Ecolog Model;* **217,** 230-239, 2008

Q.7. Bencs L, Ravindra* K, de Hoog* J, Rasoazanany* EO, Deutsch* F, Bleux* N, Berghmans* P, Roekens* E, Krata* A, Van Grieken* R; Mass and ionic composition of atmospheric fine particles over Belgium and their relation with gaseous air pollutants; *J Environm Monitor;* **10,** 1148-1157, 2008

Q.8. Lisiecki* R, Dominiak-Dzik* G, Ryba-Romanowski* W, Földvári I, Péter, Á; Energy transfer and up-conversion in Bi_2TeO_5 crystals co-doped with Yb^{3+} and Tm^{3+}; *Opt Mater;* **31**, 306-310, 2008

Q. 9. Stranger* M, Krata* A, Kontozova-Deutsch* V, Bencs L, Deutsch* F, Worobiec* A, Naveau* I, Roekens* E, Van Grieken* R; Monitoring of NO_2 in the ambient air with passive samplers before and after a road reconstruction event; *Microchem J*; accepted for publication

Q.10. Worobiec* A, Samek* L, Karaszkiewicz* P, Kontozova-Deutsch* V, Stefaniak* EA, Van Meel* K, Krata* A, Bencs L, Van Grieken* L; A seasonal study of atmospheric conditions influenced by the intensive tourist flow in the Royal Museum of Wavel castle in Cracow, Poland; *Microchem J*; accepted for publication

Q.11. Buczynska* A, Krata* A, 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; *Atmosph Environm*; accepted for publication

Q.12. Van Meel* K, Horemans* B, Bencs L, Krata* A, Buczynska* A, Dirtu* AC, Worobiec* A, Van Grieken* R; Elemental concentrations in aerosols at the Belgian coast, as a function of size, season and air mass trajectories; *Environm Chem Lett;* accepted for publication

Q.13. 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*; accepted for publication

Conference proceeding in Hungarian

Q.14. Dravecz G, Szaller Zs, Kovács L; Sztöchiometrikus $LiNbO_3$:Yb kristályok optikai spektroszkópiai tulajdonságai (Optical spectroscopy of stoichiometric $LiNbO_3$:Yb crystals, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; P-23 (1-2)

See also: M.8., M.19., R.2., R.3., R.4., R.5., R.8, R.11., R.12.

R. CRYSTAL PHYSICS AND NONLINEAR OPTICS

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

TEM studies on yttrium aluminium borate (YAB) single crystals. — Lattice defects in ion-thinned specimens of YAB single crystals were studied by transmission electron microscopic (TEM) imaging and energy dispersive X-ray spectroscopic (EDS) methods. A fine stripe structure of bright-dark contrasts with stripe widths varying between about 200 and 1500 nm was found. Between the neighbouring stripes small-angle disorientations and small compositional deviations could be detected by transmission electron diffraction and EDS, respectively.

Investigations of optical-damage-resistant $LiNbO_3$:Mg single crystals. — Light-induced absorption changes observed in the visible and near infrared spectral range upon excitation with intense nanosecond pulses of a green laser indicate the transient generation of polarons. In $LiNbO_3$ and $LiNbO_3$:Mg with doping concentrations below the optical-damage-resistance threshold these are small O^- hole polarons and bound small Nb^{4+}_{Li} electron polarons with a lifetime of ~0.4 ms. In contrast, for Mg concentrations above the threshold the light-induced absorption is caused by hole polarons and free small Nb^{4+}_{Nb} electron polarons decaying on the μs range.

In $LiNbO_3$:Mg crystals above the photorefractive threshold, the intensity of the OH^- vibrational band at about 3534 cm^{-1} decreases with increasing temperature while the band at about 3465 cm^{-1} characteristic for OH^- in undoped stoichiometric crystals emerges. The higher the Mg content, the higher the temperature where the 3465 cm^{-1} band appears. A thermal activation energy of about 0.26 eV was determined. Our results show that the same kind of defect complex known in undoped stoichiometric $LiNbO_3$ may also be formed in above-threshold $LiNbO_3$:Mg crystals due to diffusion facilitated by higher temperatures.

Spectroscopy of alkali-doped potassium lithium niobate crystals. — The effect of Na and Cs dopants on the crystal structure and composition of $K_3Li_2Nb_5O_{15}$ (KLN) has been studied by measuring the OH^- vibrational, Raman, and UV spectra and the ferroelectric Curie-temperature. In the Na-doped KLN crystals the Na^+ ions substitute for Li^+ ions while the amount of antisite Nb^{5+} ions increases resulting in the distortion of the crystal lattice. In Cs-doped KLN crystals, on the contrary, the Cs^+ ions presumably occupy the otherwise unfilled potassium sites, and decrease the number of antisite Nb^{5+} ions thereby improving the KLN crystal quality.

Spectroscopy of Cu centres in lithium tetraborate single crystals. — Time-resolved spectroscopic investigations of Cu^+ and Cu^{2+} centres in $Li_2B_4O_7$:Cu lead to a deeper understanding of the radiation induced processes underlying the applications of this material as a neutron detector and a tissue-equivalent thermoluminescent dosimeter material. A tunnelling splitting of the ground state of Cu^+ centres has been inferred from the appearance of a second luminescence decay component at low temperature. Charge captures, transferring Cu^+ to Cu^{2+} or vice versa, have accordingly to be accompanied by substantial displacements of both the dopant cation and the nearby Li^+ ions.

Hydroxyl ions in oxide crystals. — Several weak bands tentatively attributed to the stretching mode of OH^- ions incorporated during crystal growth have been observed in the

[#] Ph.D. student

optical absorption spectra of pure and rare-earth doped $YAl_3(BO_3)_4$ single crystals in the 3350 – 3650 cm^{-1} wavenumber region. An additional absorption band at about 5250 cm^{-1} at 8 K has also been detected in almost all samples. The temperature and polarization dependences of these bands, and their possible origin have been analysed.

The presence of hydroxyl ions have been detected in cadmium tungstate ($CdWO_4$) crystals by high resolution infrared absorption spectroscopy. Three main bands between 3497-3518 cm^{-1} were accompanied by several very weak lines, all attributed to hydroxyl ions in different environments. The exchange of OH^- for OD^- in heavy water vapour atmosphere has been used to calculate the anharmonicity of the stretch modes. The O-H bond directions for the different hydroxyl centres have also been determined from the spectra detected for polarized light propagating along the crystallographic axes of the monoclinic crystal.

Multiferroic materials. — Heavy rare-earth manganites, $RMnO_3$ (R = Er, Tm, Yb, Lu) with hexagonal crystal structure are ferroelectric below the Curie-temperature (T_C) and antiferromagnetic below the Néel-temperature (T_N). The optical absorption spectra in the infrared spectral range reveal the crystal field splitting of the free ion multiplets, showing also the splitting of some Kramers doublets due to magnetic ordering below T_N. The Néel-temperature has been determined for $ErMnO_3$ ($T_N \approx 76$ K) and $TmMnO_3$ ($T_N \approx 83$ K) crystals by measuring the infrared absorption spectra as a function of temperature.

Holography in photorefractive crystals. — A computer code was developed for the evaluation of the interferograms obtained by an interference microscopic study of holographic gratings in Fe-doped $LiNbO_3$ crystals. The program was used to determine the amplitude of the refractive index modulation of the phase gratings with high precision.

Design and fabrication of diffractive optical elements and waveguides by ion implantation. — Slab waveguides have been designed and fabricated in erbium doped tellurite glass samples via single step implantation of 1.5 MeV N^+ ions at an extended range (10^{12} – 10^{16} ions/cm^2) of the implanted doses, using a special silicon mask. Functionality tests (m-line spectroscopy) proved that all waveguides worked. Depending on the parameters of the implantation, a thermal annealing of the waveguides either enhanced or reduced the as-implanted refractive index modulation. To explain the fabrication process of channel waveguides a simple model based on Stopping and Range of Ions in Matter (SRIM) calculations was proposed.

History of science. — The development of the Gyulai-Tarján school of crystal physics in our days has been described and analysed.

E-Mail:

István Bányász	banyasz@szfki.hu
Gábor Corradi	corradi@szfki.hu
Ivett Hajdara	hajdara@szfki.hu
Ervin Hartmann	hartmann@szfki.hu
László Kovács	lkovacs@szfki.hu
Krisztián Lengyel	klengyel@ szfki.hu
Gábor Mandula	mandula@szfki.hu
László Malicskó	malicsko@szfki.hu
Andrea Watterich	watter@szfki.hu

Grants and international cooperations

OTKA T 047265 Photo- and neutronrefractive materials and phenomena (L. Kovács, 2004-2008)

OTKA K 60086 Spectroscopic studies of photon-induced electron transport for data handling and medical applications (G. Corradi, 2006-2009)

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, contributor L. Kovács, 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. Kovács L, Capelletti* R, Gospodinov* M; Vibrational frequencies of the impurity-centred oxygen tetrahedra in sillenites; *Vibrational Spectroscopy*; **46**, 69-75, 2008

R.2. Lengyel K, Szaller Zs, Péter Á, Polgár K, Kovács L; Microscopic and Raman spectroscopic investigation of the domain structures in $LiNbO_3$:Y:Mg crystals; *Ferroelectrics*; **368**, 3-11, 2008

R.3. Hajdara I, Lengyel K, Kovács L, Péter Á, Dravecz G, Szaller Zs; Compositional dependence and structure of hydroxyl ion defects in ferroelectric potassium lithium niobate; *Ferroelectrics*; **369**, 98-107, 2008

R.4. Corradi G, Nagirnyi* V, Kotlov* A, Watterich A, Kirm* M, Polgár K, Hofstaetter* A, Meyer* M; Investigation of Cu doped $Li_2B_4O_7$ single crystals by EPR and time-resolved optical spectroscopy; *J Phys: Condens Matter*; **20**, 025216/1-9, 2008

R.5. Conradi* D, Merschjann* C, Schoke* B, Imlau* M, Corradi G, Polgár K; Influence of Mg doping on the behaviour of polaronic light-induced absorption in $LiNbO_3$; *physica status solidi (RRL);* **2**, 284-286, 2008

R.6. Bányász I, Mandula G; Application of interference microscopy to the study of hologram build-up in LiNbO3 crystals; *Optics Communications*; **281**, 4268–4272, 2008

R.7. 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*; accepted for publication

R.8. 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*; accepted for publication

Conference proceedings

R.9. Bányász I, Berneschi* S, Fried* M, Cacciari* I, Lohner* T, Nunzi-Conti* G, Pászti* F, Pelli* S, Righini* GC, Watterich A, Zolnai* Z, Petrik P* ; Nitrogen-ion-implanted planar optical waveguides in Er-doped tellurite glass: fabrication and characterisation; In: *Optical Components and Materials V*., *San Jose, CA, USA, 19 – 24 January 2008;* Eds.: Michel J. F. Digonnet, Shibin Jiang, John W. Glesener, J. Christopher Dries, Proceedings of SPIE, Bellingham, WA, USA, **6890,** p. 68901A, 2008

R.10. Berneschi* S, Brenci* M, Nunzi-Conti* G, Pelli* S, Righini* GC, Bettinelli* M., Speghini* A., Bányász I, Fried* M, Khanh* NQ, Pászti* F, Watterich A, Leto* A., Pezzotti* G, Porporati* AA; Optical and structural characterization of Erbium-doped ion-implanted tellurite glasses for active integrated optical devices; In: *3rd International Conference on Smart Materials, Structures and Systems*, *Acireale, Italy, 7 – 14 June, 2008;* Eds.: Pietro Vincenzini, Giancarlo Righini, Advances in Science and Technology, **55**, 68-73 , 2008

R.11. 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

Conference proceeding in Hungarian

R.12. Hajdara I, Lengyel K, Péter Á, Dravecz G, Szaller Zs, Kovács L; Alkáli fémekkel adalékolt kálium-lítium-niobát kristályok spektroszkópiai tulajdonságai (Spectroscopy of alkali doped potassium lithium niobate crystals, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; P-25, 2008

Others

R.13. Hartmann Ervin: A Gyulai-Tarján kristályfizikai iskola. (The Gyulai-Tarján school in crystal physics, in Hungarian); *OTKA Magazin,* http://www.otka.hu/index.php?akt_menu=3746#top

See also: Q.2, Q.14.

S. QUANTUM OPTICS AND QUANTUM INFORMATICS

P. Ádám, J. Asbóth[#], 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. — The spatial self-organization of a Bose-Einstein condensate (BEC) in a high-finesse linear optical cavity was studied. The condensate atoms are laser-driven from the side and scatter photons into the cavity. Above a critical pump intensity the homogeneous condensate evolves into a stable pattern bound by the cavity field. The transition point has been determined analytically from a mean-field theory. We calculated the lowest lying Bogoliubov excitations of the coupled BEC-cavity system and the quantum depletion due to the atom-field coupling.

We have worked out an EIT-like process in a multi-level degenerate system. In the first step the system is prepared in a coherent superposition of two metastable degenerate states. These two states are coupled by a single circularly polarized, weak probe field to two degenerate excited states, which are coupled further to a common auxiliary state by an elliptically polarized strong coupling field. For a certain choice of the polarization of the strong coupling field the system exhibits the well-known EIT (electromagnetically induced transparency) behavior. However, for a wide range of polarization of the coupling field, the weak probe field gets amplified, hence the system acts as an amplifier. Decoherence effects and Doppler broadening are studied in detail.

Quantum information, entanglement and teleportation. — The Pólya number characterizes the recurrence of a random walk. We applied the generalization of this concept to quantum walks, based on a specific measurement scheme. The Pólya number of a quantum walk depends, in general, on the choice of the coin and the initial coin state, in contrast to classical random walks where the lattice dimension uniquely determines it. We analyzed several examples to depict the variety of possible recurrence properties. First, we showed that for the class of quantum walks driven by Hadamard tensor-product coins, the Pólya number is independent of the initial conditions and the actual coin operators, thus resembling the property of the classical walks. We provided an estimation of the Pólya number for this class of quantum walks. Second, we examined the two-dimensional Grover walk, which exhibits localization and thus is recurrent, except for a particular initial state for which the walk is transient. We generalized the Grover walk to show that one can construct in arbitrary dimensions a quantum walk which is recurrent. This is in great contrast with classical walks which are recurrent only for the dimensions d = 1 , 2. We examined the recurrence of the 2D Fourier walk. This quantum walk is recurrent except for a two-dimensional subspace of the initial states. We could provide an estimation of the Pólya number in its dependence on the initial state. The definition of the Pólya number involves measurement on the system. Depending on how measurement is included in the definition, the recurrence properties vary. We could show that in the limiting case of frequent, strong measurements one can approach the classical dynamics. Comparing various cases we found numerical indication that our previous definition of the Pólya number provides an upper limit.

Quantum information processing in semiconductor quantum interference devices. — We studied electron transport through multiterminal rectangular arrays of quantum rings in the presence of Rashba-type spin-orbit interaction (SOI) and of a perpendicular magnetic field. Using the analytic expressions for the transmission and reflection coefficients for

[#] Ph.D student

single rings we obtained the conductance through such arrays as a function of the SOI strength, of the magnetic flux, and of the wave vector k of the incident electron. We found that due to destructive or constructive spin interferences caused by the SOI, the array can be totally opaque for certain ranges of k, while there are parameter values where it is completely transparent. Spin resolved transmission probabilities showed nontrivial spin transformations at the outputs of the arrays. We placed pointlike random scattering centers between the rings, which resulted in the split of the Aharonov-Bohm peaks, and an oscillatory behavior of the conductance as a function of the SOI strength. We found that local (ring by ring) modulation of the spin orbit interaction (SOI) in arrays of quantum rings can lead to novel effects in spin state transformation of electrons. We showed that already small (3×3, 5×5) networks are remarkably versatile from this point of view: Working in a given network geometry, the input current can be directed to any of the output ports, simply by changing the SOI strengths by external gate voltages. Additionally, the same network with different SOI strengths can be completely analogous to the Stern-Gerlach device, exhibiting spatial-spin entanglement.

E-Mail:

Péter Ádám	adam@szfki.hu
János Asbóth	asboth@optics.szfki.kfki.hu
Péter Domokos	domokos@szfki.hu
Aurél Gábris	gabrisa@optics.szfki.kfki.hu
József Janszky	janszky@szfki.hu
Orsolya Kálmán	kalman@szfki.hu,
Attila Kárpáti	karpati@optics.szfki.kfki.hu
Zsolt Kis	zsolt@szfki.hu
Tamás Kiss	tkiss@optics.szfki.kfki.hu
Mátyás Koniorczyk	kmatyas@optics.szfki.kfki.hu
Zoltán Kurucz	kurucz@szfki.kfki.hu
Dávid Nagy	nagyd@optics.szfki.kfki.hu,
Viktor Szalay	viktor@szfki.hu
Gergely Szirmai	szirmai@optics.szfki.kfki.hu
Géza Tóth	toth@optics.szfki.kfki.hu,

Grants and international cooperations

OTKA T049234 Quantum optical systems and applications in quantum informatics (J. Janszky, 2005-2008)

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

OTKA T049234 Detection of multipartite entanglement in quantum optical systems (G. Tóth, 2006-2009)

TéT, Hungarian-Czech Bilateral Intergovernmental S&T Cooperation (CZ-2/2005): Quantum information and entanglement in quantum optical networks (T. Kiss, 2006-2008)

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

TéT, Hungarian-Spanish Bilateral Intergovernmental S&T Cooperation (ESP-17/2006): Quantum control (V. Szalay, 2007-2008)

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. Gábris A, Kiss T, Jex* I; Scattering quantum random-walk search with errors; *Phys Rev A*; **76**, 062315/1-10, 2007

S.2. Tóth G., Knapp* C, Gühne* U, Briegel* HJ; Optimal spin squeezing inequalities detect bound entanglement in spin models; *Phys Rev Lett*; **99**, 250405/1-5, 2007

S.3. Asboth JK, Ritsch* H, Domokos P; Optomechanical coupling in a one-dimensional optical lattice; *Phys Rev A*; **77**, 063424/1-25, 2008

S.4. Földi* P, Kálmán O, Benedict* MG, Peeters* FM; Networks of Quantum Nanorings: Programmable Spintronic Devices; *Nano Lett*; **8**, 2556-2558, 2008

S.5. Kálmán O, Földi* P, Benedict* MG, Peeters* FM; Magnetoconductance of rectangular arrays of quantum rings; *Phys Rev B*; **78**, 125306/1-10, 2008

S.6. Kiss T, Jex I* , Alber G* , Kollár* E; Properties of complex chaos in conditional qubit dynamics; *Int J Quant Inf*; **6**, 695-700, 2008

S.7. Koniorczyk M, Varga A* , Rapcan P* , Buzek V* ; Quantum homogenization and state randomization in semiquantal spin systems; *Phys Rev A*; **77**, 052106/1-11, 2008

S.8. Kurucz Z, Fleischhauer* M; Continuous-variable versus electromagnetically-induced-transparency-based quantum memories; *Phys Rev A*; **78**, 023805/1-12, 2008

S.9. Lev* BL, Vukics* A, Hudson* ER, Sawyer* BC, Domokos P, Ritsch* H, Ye* J; Prospects for the cavity-assisted laser cooling of molecules; *Phys Rev A*; **77**, 023402/1-13, 2008

S.10. Nagy D, Szirmai G, Domokos P; Self-organization of a Bose-Einstein condensate in an optical cavity; *Eur Phys J D*; **48**, 127-137, 2008

S.11. Stefanak M* , Jex I* , Kiss T; Recurrence and Pólya number of quantum walks; *Phys Rev Lett*; **100**, 020501/1-4, 2008

S.12. Stefanak M* , Kiss T, Jex I* ; Recurrence properties of unbiased coined quantum walks on infinite d-dimensional lattices; *Phys Rev A*; **78**, 032306/1-12, 2008

S.13. Tóth G; QUBIT4MATLAB V3.0: A program package for quantum information science and quantum optics for MATLAB; *Comput Phys Comm*; **179**, 430-451, 2008.

S.14. Kiss T, Kecskés* L, Stefanak* M, Jex* I; Recurrence in coined quantum walks; *Physica Scripta*; accepted for publication.

S.15. Kárpáti A, Ádam P, Janszky J; Quantum operations in probabilistic representation; *Physica Scripta*; accepted for publication

Conference proceedings in Hungarian

S.16. Ádám P, Kiss T, Janszky J, Jex* I; Schrödinger-macska állapot előállítása realisztikus kereszt Kerr-effektussal (Schrödinger-cat-state preparation by realistic Kerr-effect, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; Összefoglalók, P-18

S.17. Darázs* Z, Kiss T; Folytonos idejű kvantumos véletlen bolyongás Pólya-féle száma (The Pólya-number of the continuous time quantum walk, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; Összefoglalók, P-19

S.18. Kecskés* L, Kiss T, Stefanak* M, Jex* I; Diszkrét kvantumos bolyongás Pólya-féle száma (The Pólya number of the discrete quantum walk, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; P-29

S.19. Kollár* B, Kiss T, Stefanak* M, Jex* I; Két részecskés kvantumos bolyongás (Quantum walk of two particles, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; Összefoglalók, P-30

S.20. Nagy D, Szirmai G, Domokos P; Optikai rezonátor módusához csatolt Bose-Einstein kondenzátum átlagtérelmélete (Mean-field theory of a Bose-Einstein condensate coupled to an optical resonator, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; P-33

S.21. Kálmán O, Földi* P, Benedict* MG, Peeters* FM; Spinfüggő transzmisszió kvantumgyűrűk négyzetes rácsán (Spin-dependent transmission through rectangular arrays of quantum rings, in Hungarian); In: *Kvantumelektronika 2008, 6th National Symposium on Quantum Electronics, 17. October 2008, Budapest, Hungary*; Eds: Péter Á, Kiss T, Varró S; P-27

EDUCATION

Graduate and postgraduate courses, 2008

— Advanced solid-state physics I.-II. (J. Sólyom, ELTE[1])
— Statistical physics (F. Iglói , SZTE[2])
— Application of statistical physics (F. Iglói, SZTE)
— Disordered systems (F. Iglói, SZTE)
— Many body systems II. (P. Szépfalusy, ELTE)
— Electronic states in solids (J. Kollár, ELTE)
— Metal physics (J. Kollár, I. Tüttő, BME[3])
— Advanced solid state physics III. (I. Tüttő, ELTE)
— Solid state research I.-II. (I. Vincze, ELTE)
— Amorphous and crystalline materials (S. Kugler* and T. Kemény, BME)
— 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, ELTE)
— Physics of granular materials (J. Kertész*, T. Unger* and T. Börzsönyi, BME)
— Nanophase metals (I. Bakonyi, ELTE)
— Advanced material technology (G. Konczos, ELTE)
— Group theory in solid state research (G. Kriza, BME)
— Superconductivity (G. Kriza, BME)
— 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)
— Neutron scattering in condensed matter (L. Rosta, ME[4])

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

— Disorder in condensed phases (L. Pusztai, ELTE)
— Physics of amorphous matter I.-II. (M. Koós, SZTE)
— Experimental methods in materials science (M. Veres, BME)
— Crystal physics of optical crystals (I. Földvári, 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)
— Mechanics (P. Ádám, PTE[5])
— Quantum mechanics II. (P. Ádám, PTE)
— Mathematical methods in physics II. (P. Ádám, PTE)
— Resonant light-matter interaction (P. Ádám, PTE)
— Quantum optics (J. Janszky, PTE)
— Quantum information (J. Janszky, PTE)
— Methods in quantum information (M. Koniorczyk, PTE)
— Many-body theory (M. Koniorczyk, PTE)
— Introduction to programming (M. Koniorczyk, PTE)
— Operating systems in practice (M. Koniorczyk, PTE)
— Introduction to quantum optics (Z. Kis, ELTE)
— Coherent control of quantum systems (Z. Kis, ELTE)

Laboratory practice and seminars

— Solid-state physics seminar (J. Sólyom, ELTE)
— Seminar in quantum mechanics (B. Lazarovits, BME)
— Infrared spectroscopy laboratory practice (V. Zólyomi, ELTE)
— Advanced molecular physics laboratory practice (V. Zólyomi, ELTE)
— Laboratory for solid state physics, Preparation and crystallization of metallic glasses (I. Vincze, ELTE)
— Laboratory for solid state physics, Low-temperature magnetic measurements using a SQUID magnetometer (L.F. Kiss, ELTE)

[5] PTE = University of Pécs

— 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)

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

— 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)

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

— Advanced solid state physics laboratory (M. Bokor and G. Kriza, BME)

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

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

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

— Physics seminar (M. Koniorczyk, PTE)

Diploma works

P. Salamon (BME): Study of physical properties of banana nematic liquid crystals (Supervisor: N. Éber)

B. Tóth (ELTE): Study of spin-dependent electron transport in Ni-Co and Ni-Cr alloys (Supervisor: I. Bakonyi and L. Péter)

D. Gajári (BME): NMR study of hydrogen absorption in Pd-Ag alloys (co-supervisor: M. Bokor)

L. Szabó (PTE): Diagnostic methods of bosons trapped in optical lattices

J. Hegedüs (ELTE): The use of computers in teaching classical mechanics in high-schools

Ph. D. students

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)

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 Graduate Program in Physics): Far-infrared spectroscopy of carbon nanotubes (Supervisor: K. Kamarás)

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

L Környei (SZTE): Statics and dynamics of random-field Ising models (Supervisor: F. Iglói)

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)

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

B. Tóth (ELTE): Giant magnetoresistance (GMR) in multilayers (Supervisor: 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)

M. Fábián (ELTE): The structure of borosilicate glasses (Supervisor: E. Sváb)

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)

S. Tóth (SZTE): Light emission of carbon based films and nanoclusters (Supervisor: M. Koós)

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, Ph.D. dissertation, applied (Supervisor: P. Jani)

G. Dravecz (ELTE and Université de Metz): Study of the phase equilibria and crystal growth in the ternary system A_2O-Li_2O-M_2O_5 (A= K,Rb,Cs, M=Nb,Ta) (Supervisor: K. Polgár)

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)

Dissertations

J. Asbóth (PhD, PTE and University of Innsbruck): Interaction between optically trapped particles due to optomechanical coupling (Supervisor: P. Domokos)

D. Oszetzky (PhD, BME): Quantum optical methods in metrology (Supervisor: A. Czitrovszky)

AWARDS

— N. Kroó: Honorary Doctor of the Joint Institute for Nuclear Research, Dubna (2008)

— G. Konczos: International Prize 2008 of the Slovak Academy of Sciences

— L. Cser: Commander's Cross Order of Merit of the Hungarian Republic (civil division)

— A. Czitrovszky, Petzval Award, 2008

— Z. Kis: Pál Gombás Award of the Loránd Eötvös Physical Society

— Á. Buka: Physics Prize of the HAS

— V.M. Budea: Diploma of merit of the Secretary General, HAS

— E. Hartmann: Diploma of merit (Technical University, Budapest 2008)

— E. Hartmann: Diploma of golden jubilee (Eötvös University, Budapest 2008)

— L. Malicskó: Diploma of merit (Technical University, Budapest 2008)

— N. Éber: SZFKI Annual Publication Award (2008)

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

— T. Börzsönyi: Bolyai Grant (2005-2008)

— P. Jóvári: Bolyai Grant (2008-2011)

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

— K. Kutasi: Bolyai Grant (2008-2011)

— P. Dombi: Bolyai Grant (2007-2010)

— M. Veres, Bolyai Grant (2006-2008)

— 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: Member of the ESF Physical and Engineering Sciences Standing Committee

— 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 (Kutatási és innovációs eseti bizottság), 2007-?

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

— G. Oszlányi: member of Solid State Committee of Physical Section of HAS

— 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 Solid State Physics Committee 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: Member of the International Liquid Crystal Society, Board of Directors

— 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 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)

— L.K. Varga: Member of International Advisory Committee (2004-), Czech and Slovak Conference on Magnetism (CSMAG)

— I. Bakonyi and L.K. Varga, Members of Local Scientific Committee, International Conf. on Magnetic Measurements (Budapest, 2008)

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

— L. Péter, Secretary of Electrochemical Committee of HAS (2005-)

— G. Kriza, Member of Solid State Physics Committee of HAS (2007-2009)

— G. Kriza, Elected Member of the General Assembly of HAS (2007-2009)

— G. Kriza, Member of Ph.D. School of Physics, BME (2008-)

— K. Tompa, Member of Solid State Physics Committee of HAS (1997-2008)

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

— K. Tompa, Member of Ph.D. Council of ELTE (2008-2010)

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

— L. Rosta: Scientific Advisory Council of ILL (Institute Laue-Langevine), Grenoble, France

— 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

— 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: Member of the Int. Organizing Committee of European Aerosol Conference (Thessaloniki, 2008)

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

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

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

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

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

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

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

— L. Kovács: L. Kovács: Member of the Hungarian National Committee, International Union of Crystallography

— E. Hartmann: Member of Hungarian Language Committee of HAS (1971-2008)

— 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

— This year we have organized a Workshop on "**New challenges in the Electronic Structure of Complex Materials**" (June 29 - July 1, 2008, organized by J. Kollár and L. Vitos). The purpose of the meeting was to provide an overview on our recent activity about studying the bulk and surface electronic properties of metals and alloys, and stimulate cooperation in these fields. The meeting started on Sunday afternoon and it was closed on Tuesday noon. The number of participants was 40 from ten different countries. The programme of the workshop can be found in the web-page of our institute.

— **4th Szeged International Workshop on Advances in Nanoscience** (co-organized with the University of Szeged), October 8-10, Szeged, 150 participants Organizing committee: K. Kamarás, R. Hackl, I. Kiricsi, Z. Kónya, Á. Kukovecz.

— **The European Spallation Source (ESS)** is one of the most advanced R&D infrastructure projects of the European Union. It will be the most advanced neutron scattering facility in the world by making full use of the unique capabilities of the innovative long pulse spallation source concept introduced by Ferenc Mezei. It will provide unprecedented research potentials in many crucial areas of science and technology. Hungary has also been an active participant in the development and formation of the idea of ESS from the earliest stage. It is the firm intention of Hungary to participate in the realisation of the ESS facility and the Hungarian government is ready to finance a substantial part of ESS to be located in Debrecen, in eastern part of the country. Together with the Ministry for National Development and Economy and the ESS Hungary Co. we organised a **workshop** to promote the regional advancement of the project. The meeting was held on June 16-17, 2008 at the MTA KFKI Research Campus in Budapest and at the University of Debrecen. At the workshop the Budapest Neutron Centre and the ATOMKI facilities as well as the progress of the preparation of the ESS Hungary Project were presented with the participation of 35 experts from 8 countries, essentially from the Central European Region.

TABLE of CONTENTS