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2007

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

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ANNUAL REPORT 2007

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

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Dear Reader,

It is my pleasure to hand over the 14th, 2007 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 we gained independence as Research Institute for Solid State Physics. 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 are Research Institute for Solid State Physics and Optics.

The mission of the Institute is 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, crystal growth, and metallurgy. Since January 1, 2007 the Institute hosts the campus research library.

About 65 % 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.

Our staff of 190 includes 130 scientists. This year we have published more than 213 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 an essential role of international co-operation in our research. Two textbooks have also been published by our scientists: “Fundamentals of Physics of Solids,” Vol. 1 by Jenő Sólyom (Springer) and “Computational Quantum Mechanics for Materials Engineers” by Levente Vitos (Springer).

The achievements of our scientists have been acknowledged by several awards and nominations. Patrik Fazekas has been elected a Corresponding Member of the Hungarian Academy of Sciences. One of our senior research fellows, Kálmán Tompa has been awarded the Eötvös József Medal of Merit by the Hungarian Academy of Sciences. Two researchers, Imre Bakonyi and Péter Domokos, have become Doctors of the Hungarian Academy of Sciences (DSc). Ten young researchers have received their PhD degree.

It has become a tradition of the Institute to deliver prizes for outstanding publications and achievements in applied research. In 2007, awards have been given in both categories. The

publication prize has been won by Ferenc Borondics mainly for his papers published in the highly reputed journals Science and Nature Materials. The applied research prize has been awarded to Pavel Kamasa for the development of a complex thermophysical measurement system.

During this year, our Institute suffered a serious loss by the untimely death of two outstanding colleagues, Prof. Patrik Fazekas (62) and Csaba Hargitai (68). Patrik Fazekas was a leading expert of the theory of magnetism whose contribution to the field and his textbook "Lecture Notes on Electron Correlations and Magnetism" were highly appreciated throughout the world. Csaba Hargitai, a senior research fellow started his career as theoretical solid state physicist in the field of metal physics in the early 1960's. In the mid 1970's, he initiated the study of amorphous alloys (metallic glasses), which became the main research topic in metal physics for several decades not only in our Institute, but in several other Hungarian research institutions as well.

I hope this booklet will provide useful information to the reader. The key figures help you to get a general overview of our institute as a whole. The Annual Report contains the e-mail addresses of our scientists as well, to make it easier to get in contact with them directly. For further information please visit our home page at http://www.szfki.hu

Budapest, December 5, 2007.

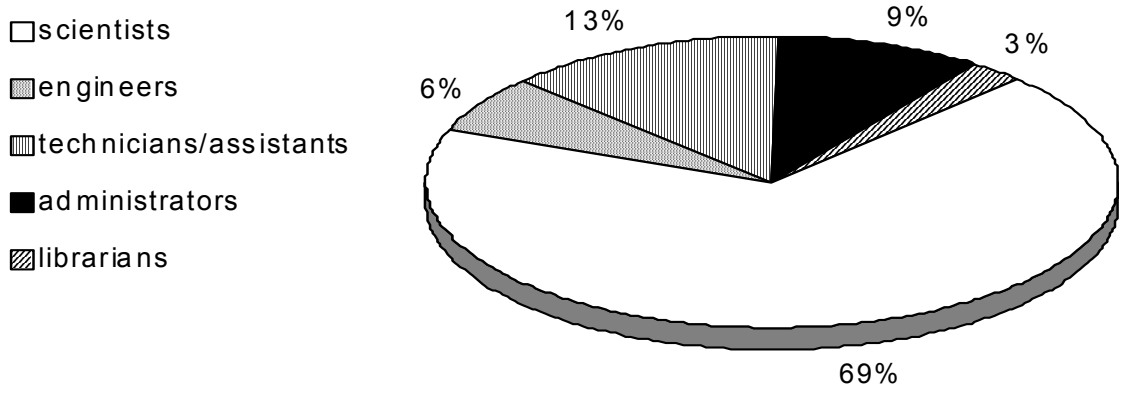
János Kollár

Director

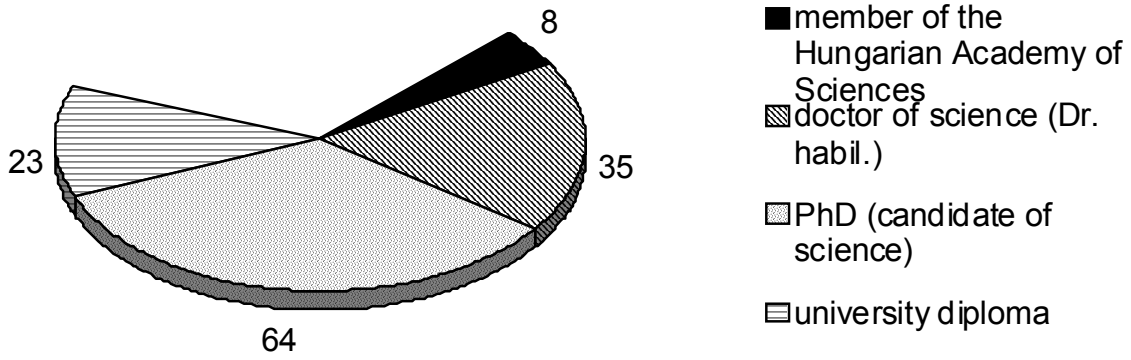
Key figures

Permanent staff of the Institute: 190 employees. Its distribution:

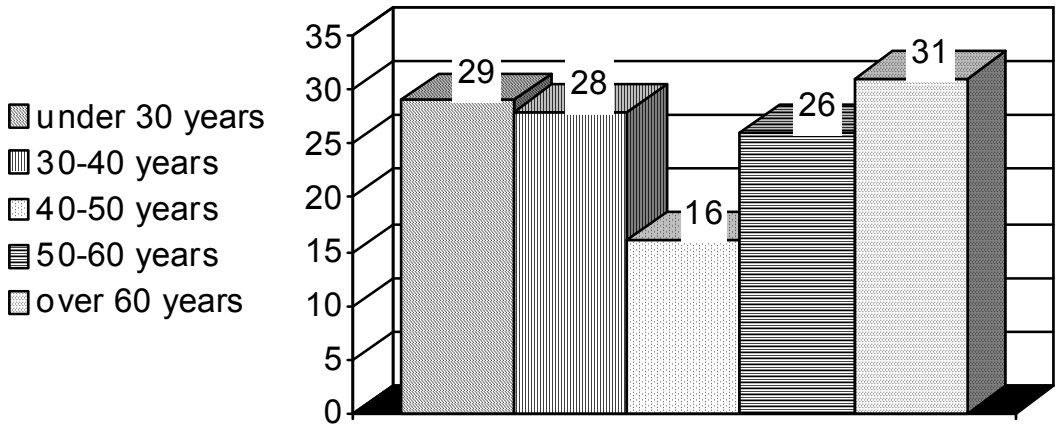
a) by professions:



b) by scientific titles/degrees:

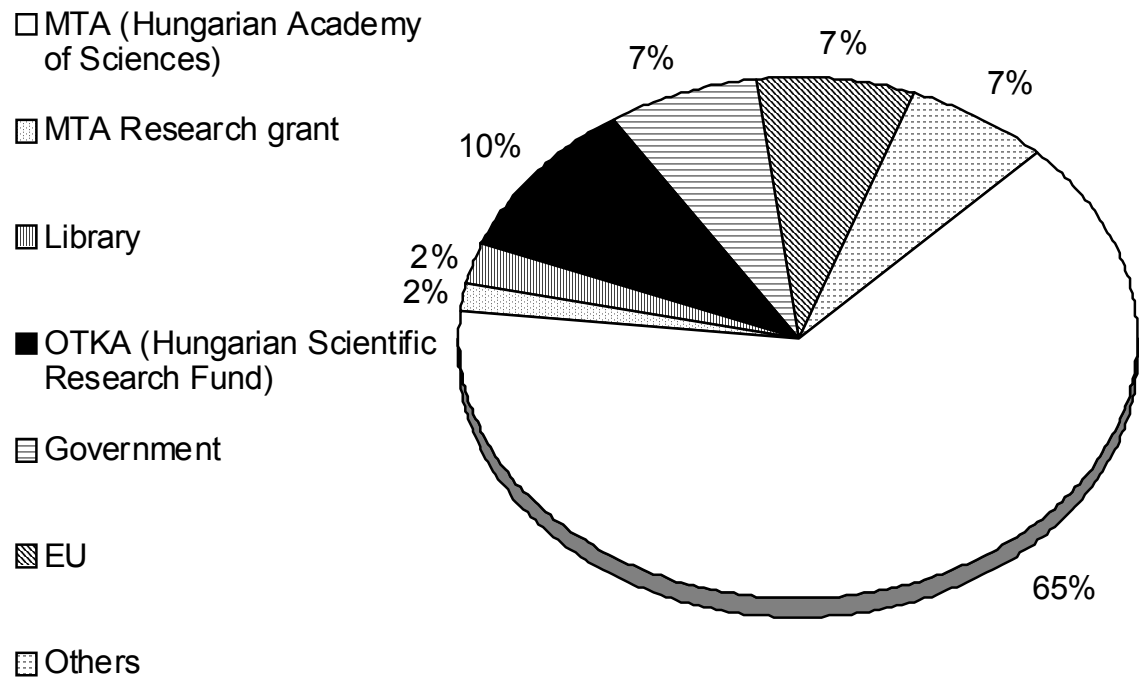


c) by ages:

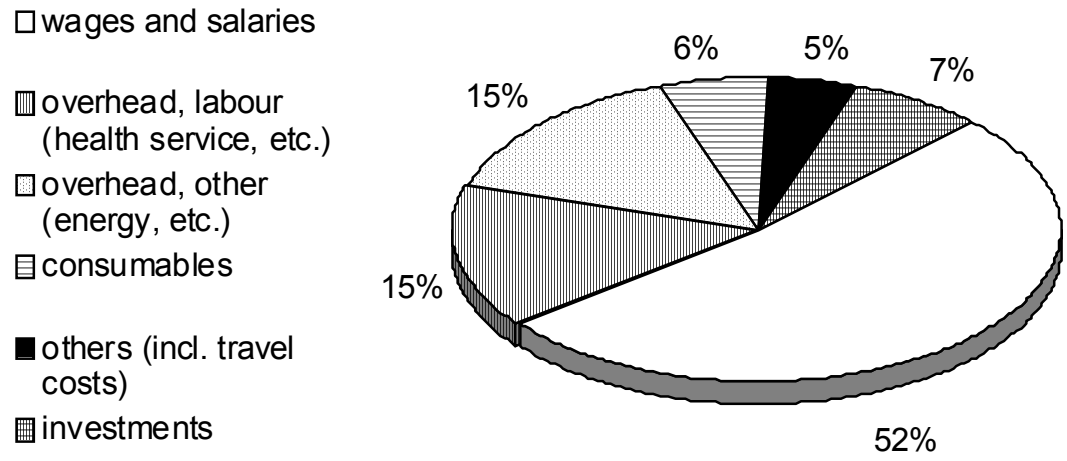


Financial management

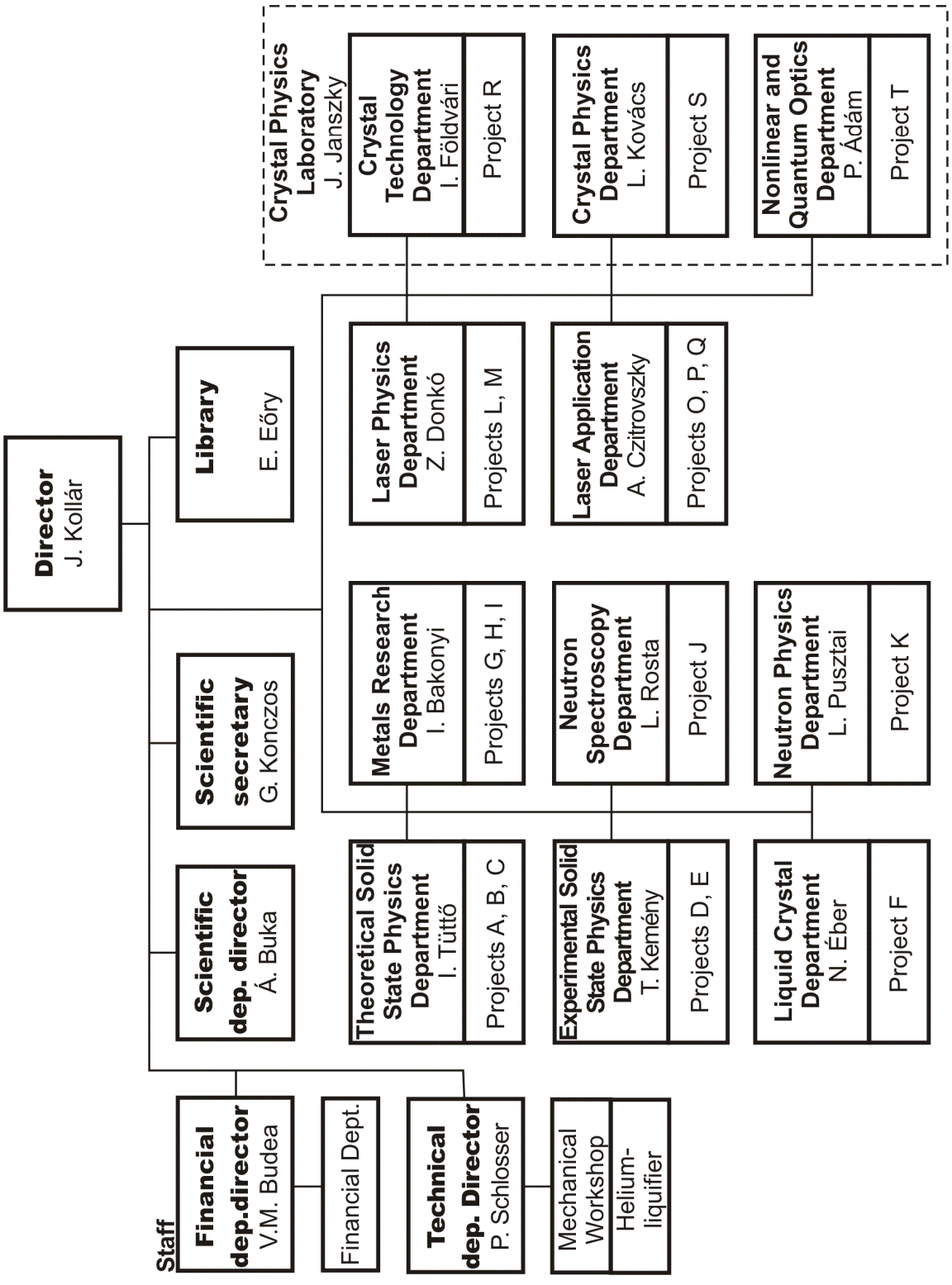
a) Sources of operation costs:



b) Distribution of expenditures:



Structure of the Research Institute for Solid State Physics and Optics



A. STRONGLY CORRELATED SYSTEMS

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

Low-dimensional fermionic models. — We have continued the study of quantum phase transitions in low-dimensional fermionic systems by analyzing the behavior of quantum-information entropies for sites and blocks calculated using the density-matrix renormalization-group (DMRG) method. We proposed a new entropy-based approach to study transitions from uniform to spatially inhomogeneous phases. It was shown that oscillations in the length-dependent von Neumann entropy and its corresponding Fourier spectrum for finite segments determine the wave vector of soft modes in critical systems, while they give the wave vector of spatial inhomogenity of the ground state in gapped systems. The phase diagram of the Hubbard model with both nearest and next-nearest hopping was determined and it was shown that the commensurate-incommensurate transition is independent of the insulator-metal transition.

By studying energy gaps and various quantum-information entropies it was shown that in the half-filled one-dimensional SU(n) Hubbard model, except for n=2, finite spin and charge gaps are found for arbitrary positive U, the transition to the gapped phase at U_c=0 is of Kosterlitz-Thouless type and is accompanied by bond dimerization both for even and odd n. In the 1/n-filled case, the transition has similar features as in the half-filled SU(2) Hubbard model. The charge gap opens exponentially slowly for $U>U_c$=0 and the spin sector remains gapless. The model was further investigated analytically by bosonization approach and numerically using the DMRG method for n=3, 4, and 5 for commensurate fillings $f=p/q$ where p and q are relatively prime. Umklapp processes are irrelevant when $q>n$, and the model is equivalent to an n-component Luttinger liquid with central charge $c=n$. When $q=n$, the charge and spin modes are decoupled, umklapp processes open a charge gap for finite $U>0$, whereas the spin modes remain gapless and the central charge $c=n-1$. The translational symmetry is not broken in the ground state for any n. On the other hand, when $q<n$, the charge and spin modes are coupled, the umklapp processes open gaps in all excitation branches, and a spatially nonuniform ground state develops. Bond-ordered dimerized, trimerized or tetramerized phases are found depending on the filling.

The extended Hubbard model with on-site and next-neighbor Coulomb interaction has been studied with DMRG by calculating various quantum-information entropies. It was shown that a bond-ordered wave (BOW) phase exists between the charge-density wave (CDW) and spin-density wave phases. The transition between the CDW and BOW phases changes from first to second order before the tricritical point is reached.

We have also extended the DMRG code to carry out numerical renormalization-group (NRG) type calculations in order to apply it to quantum impurity problems. The new DMRG-NRG code has been used to study the symmetric Anderson model and a benchmark test compared with respect of the DM-NRG method has been carried out.

In a review we have shown that cross-fertilization between quantum-information theory and solid-state physics has led to improvements in our understanding of interacting quantum systems in general and the DMRG method in particular. It has led to new algorithms related to and generalizing the DMRG, and has opened up the possibility of studying many new physical problems, ones of interest both for quantum-information

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theory and for understanding the behavior of strongly correlated quantum systems. We have discussed relevant concepts in quantum-information theory, including the relation between DMRG, data compression, and entanglement.

Low-dimensional and frustrated magnetic systems. — Spin ladders have played an important role in the field of strongly correlated systems over the past decade. They are among the best studied spin-gap systems, thanks to the numerous experimental realizations in transition metal oxides and organometallic compounds; their intermediate phase in a magnetic field is one of the simplest realizations of a Luttinger liquid and frustrating them with diagonal rungs opens a magnetization plateau at half-saturation, a simple example of noninteger magnetization plateaux. All this is true for purely SU(2) Heisenberg interactions, but in actual systems, anisotropic terms such as the Dzyaloshinskii-Moriya (DM) interaction is often present. We have studied the problem using several techniques: variation with site factorized wave function, DMRG, and exact diagonalization. Our investigation has shown that even weak DM interactions can substantially modify the phase diagram of spin-1/2 Heisenberg ladders in a magnetic field provided that they compete with exchange. For non-frustrated ladders, they induce a local magnetization along the DM vector that turns the gapless intermediate phase into an Ising phase with broken translational symmetry. For frustrated ladders, they extend the Ising order of the half-integer plateau to the surrounding gapless phases of the purely Heisenberg case. Beyond ladders, we expect to find similar effects in higher-dimensional models of coupled spin-1/2 dimers, whenever DM and exchange compete. In fact, the broken translational symmetry above the 1/8 plateau of $SrCu_2(BO_3)_2$ might be an example of the frustrated case, and the ordered intermediate phase of $Cu_2(C_5H_{12}N_2)_2C_{14}$ of the unfrustrated one, at least at a qualitative level.

We have studied various two-leg spin ladders using an analytic renormalization-group method and the DMRG algorithm. We have shown that frustration generated by inter-leg couplings could lead to a new phase with columnar dimer order depending on the symmetries of the system. The operator content of the RG has been investigated in detail in the weak-coupling limit using bosonization.

Recent numerical investigations has shown that some frustrated two-dimensional systems with four-site ring-exchange processes can support nonmagnetic nematic and triatic order, which break the O(3) spin symmetry. To gain an insight into these phases, we have systematically searched for the possible order parameters of spin-1/2 systems on a triangular lattice. Beyond the usual magnetic order parameters, we found nonmagnetic nematic (quadrupolar) and triatic (octopolar) operators, which we classified according to the irreducible representations of the point group and time-reversal symmetries. These order parameters serve as a starting point towards constructing a mean-field-like theory of nonmagnetic long-range-ordered phases.

Other problems. — The spinless resonant-level model was studied when it is coupled by hopping to one of the arbitrary number of conduction-electron channels while the Coulomb interaction acts between the electron on the impurity and in the different channels. In case of repulsive or attractive interaction, the conduction electrons are pushed away or attracted to ease or hinder the hopping by creating unoccupied or occupied states, respectively. In the screening of the hopping, orthogonality catastrophe plays an important role. At equilibrium in the weak- and strong-coupling limits, the renormalizations are treated by perturbative, numerical, and Anderson-Yuval Coulomb gas methods. In the case of two leads the current due to applied voltage is treated in the weak-coupling limit. The

presented detailed study should help to test other methods suggested for nonequilibrium transport.

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Grants

OTKA* T043330	Theoretical study of strongly correlated low-dimensional systems (J. Sólyom, 2003–2007)
OTKA F046356	Development and application of the momentum-space density-matrix renormalization group method for fermionic systems (Ö. Legeza, 2004–2007)
OTKA T047003	Statistical physics of evolutionary games (Participant: G. Fáth, Ö. Legeza, 2004–2007)
OTKA T049607	Exotic phases and excitation in frustrated electron systems with charge, spin and orbital degrees of freedom (K. Penc, 2005–2007)
NKFP 2/051/2004	Language Miner (Participant: G. Fáth, Ö. Legeza, 2005–2007)
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)

Publications

Articles

A.1. Buchta K, Legeza Ö, Szirmai E, Sólyom J; Mott transition and dimerization in the one-dimensional SU(*n*) Hubbard model; *Phys Rev B;* **75**, 155108/1-10, 2007

A.2. Legeza Ö, Sólyom J, Tincani* L, Noack* RM; Entropic analysis of quantum phase transitions from uniform to spatially inhomogeneous phases; *Phys Rev Lett;* **99**, 087203/1-4, 2007

A.3. Penc K, Fouet* JB, Miyahara* S, Tchernyshyov* O, Mila* F; Ising phases of Heisenberg ladders in a magnetic field; *Phys Rev Lett;* **99**, 117201/1-4, 2007

A.4. Poilblanc* D, Penc K, Shannon* N; Doped singlet-pair crystal in the Hubbard model on the checkerboard lattice; *Phys Rev B;* **75**, 220503(R)/1-4, 2007

* OTKA = Hungarian Scientific Research Fund

A.5. Penc K, Shannon* N, Motome* Y, Shiba* H; Symmetry considerations on the magnetization process of the Heisenberg model on the pyrochlore lattice; *J Phys Condens Matter;* **19**, 145267/1-9, 2007

A.6. Borda* L, Vladár K, Zawadowski A; Theory of a resonant level coupled to several conduction electron channels in equilibrium and out-of-equilibrium; *Phys Rev B;* **75**, 125107/1-9, 2007

A.7. Szirmai E, Legeza Ö, Sólyom J; Spatially nonuniform phases in the one-dimensional SU(*n*) Hubbard model for commensurate fillings; accepted for publication; cond-mat/07083799

Conference proceeding

A.8. Shannon* N, Ueda* H, Motome* Y, Penc K, Shiba* H, Takagi* H; Half-magnetization plateaux in Cr spinels; *J Phys Conf Ser*; **51**, 31-38, 2006

Book, book chapter

A.9. Legeza Ö, Noack* R. M, Sólyom J, and Tincani* L; Applications of Quantum Information in the Density-Matrix Renormalization Group; In: *Lecture Notes in Physics;* Springer-Verlag Berlin Heidelberg, accepted for publication

A.10. Sólyom J; Fundamentals of the Physics of Solids, Volume 1 – Structure and Dynamics; Springer, Berlin Heidelberg; 2007

See also: C.25., C.26.

B. COMPLEX SYSTEMS

F. Iglói, R. Juhász, 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 behaviour. — We have studied the ferromagnetic large-q state Potts model in complex evolving networks, which is equivalent to an optimal cooperation problem, in which the agents try to optimize the total sum of pair cooperation benefits and the supports of independent projects. The agents are found to be typically of two kinds: a fraction of m (being the magnetization of the Potts model) belongs to a large cooperating cluster, whereas the others are isolated one man's projects. It is shown rigorously that the homogeneous model has a strongly first-order phase transition, which turns to second-order for random interactions (benefits), the properties of which are studied numerically on the Barabási-Albert network. The distribution of finite-size transition points is characterized by a shift exponent, $1/\widetilde{\nu}' = 0.26(1)$, and by a different width exponent, $1/\nu' = 0.18(1)$, whereas the magnetization at the transition point scales with the size of the network, N, as:$m \sim N^x$, with $x = 0.66(1)$.

Large-scale Monte Carlo simulations were used to explore the effect of quenched disorder on one-dimensional kinetic Ising models with locally broken spin symmetry. The model was found to exhibit a continuous phase transition to an absorbing state. The associated critical behavior is similar to that arising in the one-dimensional contact process with Griffiths-like behavior. Variable cluster exponents were also found which obey the hyperscaling law.

The dynamics and the structure factor of the helix-coil transition in the Poland-Scheraga model of DNA-denaturation were studied. A universal scaling behavior was found in the vicinity of the transition point, even when the transition is of first order. Predictions of Langevin dynamics for the order parameter were shown to be in agreement with the results of an evolution based on a microscopic dynamics and followed by Monte Carlo method.

In the leading order of the large N expansion to the SU(2) × O(N) globally symmetric renormalizable scalar field theory symmetry-breaking solutions are found numerically even when all fields have positive renormalized square mass. The symmetry breaking, radiatively induced by the N-component hidden phantom field, can reproduce the standard range of the electroweak condensate and of the Higgs mass.

In a one-loop parametrization of the $SU(3)_L \times SU(3)_R$ chiral quark model chiral perturbation theory for mesons and baryons is used to study the boundary of the first order phase transition region in the $m_\pi - m_K - \mu_B$ space. The boundary surface of second order phase transition points bends with increasing μ_B towards the physical point of the mass plane. At this point the scaling region of the critical end point (CEP) is explored.

Quantum systems. — We have studied the entanglement entropy of inhomogeneous quantum systems. For the two-dimensional random transverse Ising model the entanglement entropy is studied with a numerical implementation of the strong disorder renormalization group. The asymptotic behavior of the entropy per surface area diverges at, and only at, the quantum phase transition that is governed by an infinite randomness fixed point. Here we identify a *double-logarithmic* multiplicative correction to the area law for the entanglement entropy. This contrasts with the pure area law valid at the infinite randomness fixed point in the diluted transverse Ising model in higher dimensions. We

have also studied entanglement in non-periodic (quasi-periodic or more generally aperiodic) critical Heisenberg, XX and quantum Ising spin chains. For marginal and relevant aperiodic modulations, the entanglement entropy is found to be a logarithmic function of the block size with log-periodic oscillations. The effective central charge, c_{eff}, defined through the constant in front of the logarithm may depend on the ratio of couplings and can even exceed the corresponding value in the homogeneous system. In the strong modulation limit, the ground state is constructed by a renormalization group method and the limiting value of c_{eff} is exactly calculated. Keeping the ratio of the block size and the system size constant, the entanglement entropy exhibits a scaling property, however, the corresponding scaling function may be nonanalytic.

We have investigated the trapped Fermi gas at the Feshbach resonance where certain universal properties of the system have been known. We have shown that the inhomogeneity of the density and of the gap function brings in further universal numbers. They have been determined within the BCS-Leggett model.

Other researches. — Further improvements of the charge flipping (CF) method of crystallographic phase retrieval, introduced in 2004, were obtained. The method was extended to analyze neutron diffraction data which differ from those of X-ray crystallography by leading to negative scattering densities, namely for hydrogen atoms. New methods accelerating convergence have been introduced.

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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)

DAAD-MÖB 26/2006 Statistical physics of nonequilibrium and disordered systems (F. Iglói, 2006-2007)

KPI Öveges grant ASEP1111 Transport and condensation in interacting and reacting systems (F. Iglói, 2006-2007)

ESF Programme: Quantum Degenerate Dilute System (P. Szépfalusy is member of the Steering Committee)

Publications

Articles

B.1. Juhász R, Santen* L, Iglói F; Partially asymmetric exclusion processes with sitewise disorder; *Phys Rev E*; **74**, 061101/1-10, 2006

B.2. Csordás* A, Szőke* E, Szépfalusy P; Cluster states of Fermions in the single 1-shell model; *Eur Phys J D*; **42**, 113-124, 2007

B.3. Kis-Szabó* K, Szépfalusy P, Szirmai* G; Phases of a polar spin-1 Bose gas in a magnetic field; *Phys Lett A*; **364**, 362-367, 2007

B.4. Környei* L, Iglói F; Geometrical clusters in two-dimensional random-field Ising models; *Phys Rev E*; **75**, 011131/1-6, 2007

B.5. Iglói F, Juhász R, Zimborás* Z; Entanglement entropy of aperiodic quantum spin chains; *Europhys Lett*; **79**, 37001/1-6, 2007

B.6. Lin* YC, Iglói F, Rieger* H; Entanglement entropy at infinite randomness fixed points in higher dimensions; *Phys Rev Lett*; **99**, 147202/1-4, 2007

B.7. Iglói F, Lin* YC, Rieger* H, Monthus* C; Finite-size scaling of pseudo-critical point distributions in the random transverse-field Ising chain; *Phys Rev B*; **76**, 064421/1-5, 2007

B.8. Karsai* M, Anglès d'Auriac* JCh, Iglói F; Rounding of first-order phase transitions and optimal cooperation in scale-free networks; *Phys Rev E*; **76**, 041107/1-7, 2007

B.9. Pleimling* M, Iglói F; Nonequilibrium critical relaxation at a first-order phase transition point; *Europhys Lett*; **79**, 56002/1-6, 2007

B.10. Juhász R; Weakly coupled, antiparallel, totally asymmetric simple exclusion processes; *Phys Rev E*; **76**, 021117/1-13, 2007

B.11. Juhász R, Zimborás* Z; Entanglement entropy in aperiodic singlet phases; *J Stat Mech*; P04004/1-18, 2007

B.12. Kunz* H, Livi* R, Sütő A; The structure factor and dynamics of the helix-coil transition; *J Stat Mech*; P06004/1-22, 2007

B.13. Menyhárd N, Ódor* G; One-dimensional spin-anisotropic kinetic Ising model subject to quenched disorder; *PhysRev E*; **76**, 021103/1-9, 2007

B.14. Csordás* A, Almásy* O, Szépfalusy P; New universal quantities characterizing inhomogeneous Fermi gases at the Feshbach resonance; Europhys Lett; **80**, 50002/1-6, 2007

B.15. Patkós* A, Szép Zs; Phase structure and phase transitions of the SU(2) × O(n) symmetric scalar field theory; *Europhys Lett*; **79,** 51001/1-6, 2007

B.16. Kovács* P, Szép Zs; The critical surface of the $SU(3)_L \times SU(3)_R$ chiral quark mode at non-zero baryon density; *Phys Rev D*; **75**, 025015/1-10, 2007

B.17. Herpay* T, Szép Zs; The boundary of the first order chiral phase transition in the m_π - m_K plane with a linear sigma model; *Nucl Phys A***; 785**, 174-177, 2007

See also E.15.

C. ELECTRONIC STATES IN SOLIDS

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

Traditionally, new materials have been developed by empirically correlating their chemical composition, and the manufacturing processes used to form them, with their properties. Until recently, metallurgists have not used quantum theory for practical purposes. However, the development of modern density functional methods means that today, computational quantum mechanics can help engineers to identify and develop novel materials. Besides, we demonstrate that computational modeling based on modern first-principles alloy theory can yield fundamental physical parameters with high accuracy. We illustrate this in a few examples.

Using first-principles quantum-mechanical theory, we demonstrate that the surface chemistry of **Fe-Cr alloys** follows the peculiar threshold behavior characteristic to ferritic stainless steels. We find 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.

Using density-functional theory formulated within the framework of the exact muffin-tin orbitals method, we investigate the **stability of the body-centered-cubic phase of Be** (β-Be). The elastic constants and Debye temperature of β-Be are calculated over a wide volume range and compared to those obtained for the low temperature hexagonal phase (α-Be). A significant difference in the anisotropy of the bcc and hcp structures is found. In line with experiments, we predict that the hcp→bcc phase transition occurs at 240 GPa at 0 K and 239 GPa at ambient temperature. We find that the cubic shear constant $C'=(C_{11}-C_{12})/2$ rapidly decreases for volumes above $\sim 1.05V_0$, where V_0 is the zero temperature equilibrium volume for β-Be. At $1.17V_0$, the stability condition $C'>0$ is violated and the bcc phase becomes mechanically unstable. We demonstrate that at 0 K, the softening of β-Be near its experimental volume of $1.063V_0$ is related to an electronic topological transition due to the increased number of occupied *s* states near the Fermi level compared to that at V_0. This softening turns out to be important for the stability of the bcc phase before melting. The disclosed electronic topological transition is found to be present in other analogous hexagonal metals as well.

First-principles calculations show that measured **surface core-level shifts** (SCLSs) of the **GaAs(100)(2x4) surfaces** can be described within the initial state effects. The calculated As 3*d* and Ga 3*d* SCLSs for the β2 and α2 reconstructions of the GaAs(100) (2x4) surfaces are in reasonable agreement with recent measurements. In particular, the results confirm that both the lower and the higher binding energy SCLSs, relative to the bulk emission in the As 3*d* photoelectron spectra, are intrinsic properties of the GaAs(100) (2x4) surfaces. The most positive and most negative As shifts are attributed to the third layer As atoms, which differs from the previous intuitive suggestions. In general, calculations show that significant SCLSs arise from deep layers, and that there are more than two SCLSs. Our previously measured As 3*d* spectra are fitted afresh using the calculated SCLSs. The intensity ratios of the SCLSs, obtained from the fits, show that as the heating temperature of the GaAs(100) (2x4) surface is increased gradually, the area of

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the $\alpha 2$ reconstruction increases on the surface, but the $\beta 2$ phase remains within the whole temperature range, in agreement with previous experimental findings. Our results show that the combination of the experimental and theoretical results is a prerequisite for the accurate analysis of the SCLSs of the complex reconstructed surfaces.

The **surface core-level binding-energy shift of Pd** at the $Ag_cPd_{1-c}(111)$ surface is 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 are evaluated within the $Z+1$ approximation. The results are analysed using the mixing enthalpy of the alloy and the bulk and surface chemical potentials. A relation of the SCLS to the bulk concentration is considered. This relation is shown to be mediated by the surface concentration profile which induces the observed nonlinear behaviour. The results are interpreted using a simple model for the alloy electronic structure.

We have performed first principles calculations with the density functional theory based VASP code to study the **vibrational properties of various carbon nanostructures**. In detail, the following topics were investigated:

We calculated the Raman active longitudinal optical (LO) frequencies for carbon oligoynes and polyyne. We introduced a linear/exponential scaling scheme based on the exponential behavior of the carbon-carbon bond stretching force constant couplings in quasi-one-dimensional conjugated chains. This novel scaling scheme was found to yield frequencies that agree well with experimental results on long linear carbon chains encapsulated inside multiwalled or double walled carbon nanotubes. Vibrational modes of ^{13}C isotope enriched single walled carbon nanotubes are inhomogeneously broadened due to the random distribution of isotopes. We studied this effect on the radial breathing mode theoretically and compared the result with experiments on inner tubes in double walled carbon nanotubes grown from ^{13}C-enriched fullerenes. We have found evidence of the absence of carbon diffusion along the tube axis during inner tube growth, supporting the theory of inner tube growth by Stone-Wales transformations from interconnected fullerenes. The energy dispersion of the D* (G') band shows a strong diameter dependence according to Raman measurements on double walled carbon nanotubes, with the Raman shift of the small diameter inner tubes showing an average softening. We have shown that the experimental observation can be reproduced by simple model calculations if the curvature effects are taken into account. The phonon softening with increasing curvature was proven by first principles calculations.

We performed ab-initio calculations of the magnetic moments and magnetic anisotropy energies of **small FeCo clusters** of varying composition on top of a Cu(100) substrate. Three different cluster layouts have been considered, namely 2X2, 3X3 and cross-like pentamer clusters. The ratio of Co atoms with respect to the total number in a chosen cluster (”concentration”) was varied and all possible arrangements of the atomic species were taken into account. Calculations have been performed fully relativistic using the embedded-cluster technique in conjunction with the screened Korringa-Kohn-Rostoker method and the magnetocrystalline anisotropy energy (MAE) has been evaluated by means of the magnetic force theorem. A central result of the investigations is that the size of the magnetic moments of the individual Fe and Co atoms and their contributions to the anisotropy energy depend on the position they occupy in a particular cluster and on the type and the number of nearest-neighbors. The MAE for the 2X2 and 3X3 clusters varies with respect to the „concentration” of Co atoms in the same manner as the corresponding monolayer case, whereas the pentamer clusters show a slightly different behavior.

Furthermore, for the clusters with an easy axis along a direction in the surface plane, the MAE shows a significant angular dependence.

We have continued to investigate theoretically various properties of **unconventional density waves** (UDW) in quasi one, and two dimensional systems. Our calculations of the pseudogap enhancement in d-density waves due to magnetic impurities are in qualitative agreement with recent experimental data on the nickel substituted NBCO high-T_c superconductor. This lends further support to our claim, that the pseudogap phase of underdoped high-T_c superconductors is an UDW. We have worked out the theory of a single nonmagnetic impurity placed in an UDW host. Both the local density of states and the Friedel oscillations show unambiguous charasterictics of an UDW. Due to the presence of low energy excitations, the Friedel oscillations extend much farther from the impurity than in conventional density waves, facilitating experimental observation. We also considered a macroscopic number of randomly distributed nonmagnetic impurities in the presence of UDW, and determined the thermodynamics of the system for arbitrary scattering rate. Our results bridge the gap between calculations in the Born, and in the unitary limit.

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Grants and international cooperations

OTKA T048827	First principles calculations for surfaces; surface stress and segregation (J. Kollár, 2005-2008)
OTKA T046773	Investigation of metals, alloys and oxides using the density functional theory (L.Vitos, 2004-2007)
OTKA K62280	Phase transitions in correlated electron systems: Theory and NMR experiments (P. Fazekas , 2006-2009)
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)
EFS Programme:	Towards atomistic materials design (J. Kollár, 2003-2007)

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D. NON-EQUILIBRIUM ALLOYS

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

Perpendicular Anisotropy in Fe-Ag Multilayers. — The direction of the spontaneous magnetization was observed in our previous studies to change from in plane to out of plane below 1 nm Fe layer thickness in Fe-Ag multilayers. This transition is studied in more details on a set of samples with the following structure: $[Ag(2.6\ nm)/\ ^{57}Fe(x\ nm)]_{10}$ ($0.2 \leq x \leq 1$). The samples were prepared on room temperature Si(111) substrates by vacuum evaporation. For transmission Mössbauer spectroscopy measurements they were capped with a thick capping layer (55 nm Ag and 100 nm B) and the deposited layers were removed from the substrate by using scotch tape. The stress arising because of the application of a thick capping layer and the removal of the samples from the substrate was shown to have negligible effect on the spontaneous magnetization by comparing the results to conversion electron Mössbauer spectroscopy measurements of samples on the Si substrate with a thin, 5 nm Ag, capping layer.

The samples show superparamagnetic behavior in the whole Fe thickness range. This is indicated by the deviation of the field cooled (FC) and zero field cooled (ZFC) magnetization curves measured by a SQUID magnetometer, as shown in Fig. 1 for a few representative samples. The blocking temperature, as defined by the temperature of the maximum in the ZFC magnetization, is 34 K for x=0.2 and rapidly increases with increasing x until x=0.5. The broadening of the distribution in the size of the superparamagnetic grains with increasing x can also be inferred from the ZFC curves. Samples with $x \geq 0.6$ are also superparamagnetic, as it is indicated by in-field Mössbauer measurements (not shown here), but for the majority of the Fe atoms the blocking temperature (T_B) is well above room temperature. The low temperature anomaly of the FC-ZFC curves of these samples (for x=0.7 see Fig. 1) can be attributed to an about 10-20% of the Fe atoms forming smaller grains with T_B below room temperature.

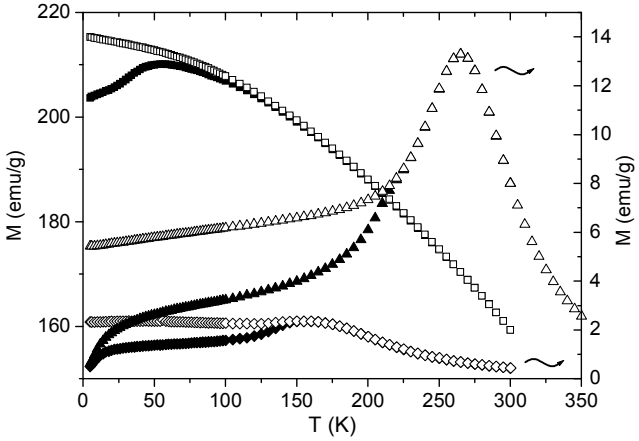

Fig. 1. *Temperature dependence of the magnetization of the x=0.4 (diamonds), 0.5 (triangles), and 0.7 (squares) [Ag(2.6 nm)/ ^{57}Fe(x nm)]$_{10}$ samples measured in 10 Oe magnetic field after cooling the sample in zero (full symbols) and 10 Oe (open symbols) applied field. Note the smaller magnetization scale for x=0.4 and 0.5.*

The direction of the spontaneous magnetization was studied by Mössbauer spectroscopy. The intensity of the 2nd and 5th lines (I_{25}) of a magnetic sextet with respect to that of the 3rd and 5th lines is determined by the angle (θ) between the direction of the local magnetization and of the γ-ray, $I_{25}=4\ \sin^2\theta\ /\ (1+\cos^2\theta)$ During a perpendicular to in-plane transition of the magnetization I_{25} changes from 4 to zero. In the case of a hyperfine field distribution an average value of I_{25} can be given by supposing a uniform direction of all the magnetic moments. The I_{25} amplitudes determined in a broad temperature range below T_B for several samples are shown in Fig. 2. A significant change of the magnetization

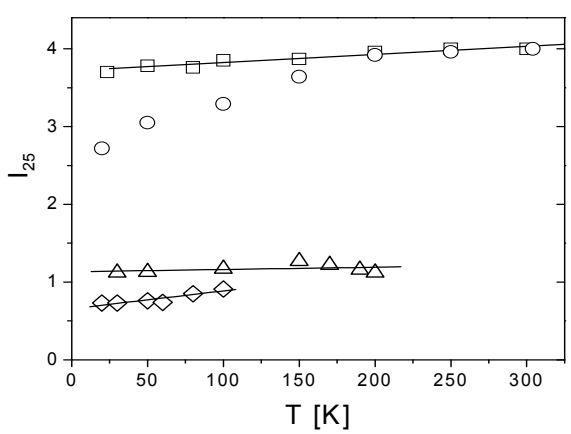

***Fig. 2**. Average intensity of the 2nd and 5th lines of the magnetic components as a function of temperature for the x=0.4 (diamonds), 0.5 (triangles), 0.6 (circles), and 0.7 (squares) [Ag(2.6 nm)/ ^{57}Fe(x nm)]$_{10}$ samples.*

direction occurs around x=0.6. It should be noted that for each sample the spectra were evaluated as a sum of magnetic and non-magnetic components, the ratio of latter gradually decreasing with decreasing temperature. For samples of x=0.4, 0.5, and 0.7, a slight decrease of the average I_{25} of the magnetic components can be observed with decreasing temperature. It hardly exceeds the uncertainty arising from the correlation of line width and amplitude values and might be due to stress induced by heat dilatations of the different layers. Nevertheless, the observed temperature dependence cannot explain the rather sharp change in the anisotropy direction as a function of layer thickness. The largest temperature variation of I_{25} is observed below 150 K for x=0.6, which is probably close to the width where the crossover between the anisotropy directions occurs and that way the most effected by thickness fluctuations of the layers.

These studies undoubtedly show that the appearance of the perpendicular anisotropy at around x=0.6 is an intrinsic property of our Fe-Ag multilayers. It is not due to the stress arising from the temperature variation, application of a capping layer or the sample removal process. Our preliminary results on granular alloys of similar Fe concentration and blocking temperature prepared by co-evaporation of the elements indicate that the out of plane spontaneous magnetization is related to the layered structure.

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Grants and international cooperations

OTKA T 048965 Magnetic properties of multilayer structures (J. Balogh, 2005-2008)
OTKA T046795 Superferromagnetism in nanostructures (I. Vincze, 2004-2007)
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)

Publications

Articles

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See also H.6.

E. X-RAY DIFFRACTION

G. Faigel, F. Borondics[#], G. Bortel, B. Botka[#], L. Gránásy, A. Jánossy[+], 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

Fullerenes and related systems. — 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 types 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. Our group studied these two types of fullerene based materials.

We have investigated the alkali fulleride materials by infrared spectroscopy and determined the spectra in the dynamic Jahn-Teller state of the divalent and tetravalent fulleride ion. We found that the special movement of the fullerene balls, pseudorotation, overcomes the distorting effect of the cations in solid salts at high enough temperature. We also determined the vibrational properties of cubane-fullerene cocrystals and the products of their copolymerization either by heat or by photons. Based on vibrational (infrared and Raman) spectra and subsequent symmetry analysis, we proposed a linear structure for the copolymers.

In connection to fullerene-cubane type materials we investigate two more points, which is 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. Recent studies suggest that the rotor-stator properties depend on the shapes and sizes of the constituents, and the new materials compose a series of orientational mesomorphic phases in between the orientationally ordered and the plastic cocrystals. In the framework of international collaborations we also performed the copolymerization of the fullerene-cubane materials under photochemical conditions and at high pressures.

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 studied the optical and thermal properties of transparent nanotube films, in their pristine form and modified by chemical functionalization. We found both optical and Raman spectroscopy useful in characterizing the degree of functionalization of these materials.

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Ab initio structure solution. — In recent years we have developed an *ab initio* method of crystal structure determination – named charge flipping (CF). The algorithm is iterative and works in dual spaces. Its operation is based on weak perturbations of low electron density. Such a working principle radically differs from that of classical direct methods, and offers complementary applications. Charge flipping can also be used at different stages of the structure solution process. It can either operate in a truly *ab inito* manner, without utilizing any preliminary structural information, or can be applied to complete a partially known structure or phase set, it can check the stability of a solution, but it can also be adapted to work as an ingredient of other dual-space schemes. Although positivity was thought to be a crucial precondition for the CF algorithm, recently we have investigated how well the presence of negative scattering density can be tolerated. For this purpose we have introduced the band flipping version of the basic algorithm, and found that the basic+band combination allows the solution of structures using neutron diffraction data alone. Initially, these results were thought to be only of theoretical interest, but with more intense neutron sources in sight, it is likely that *ab inito* neutron crystallography shall become more widespread in practice and such an algorithm may be applied.

Theory of phase transformations. — A phase field (PF) approach has been developed to model wetting and heterogeneous crystal nucleation of an undercooled pure liquid in contact with a sharp wall. Various choices for the boundary condition at the wall have been discussed and we determined the properties of critical nuclei, including their free energy of formation and the contact angle as a function of undercooling. We have found that with particular choices of boundary conditions, we may realize either an analog of the classical spherical cap model or a decidedly non-classical behavior, where the contact angle decreases from its value taken at the melting point towards complete wetting at a critical undercooling.

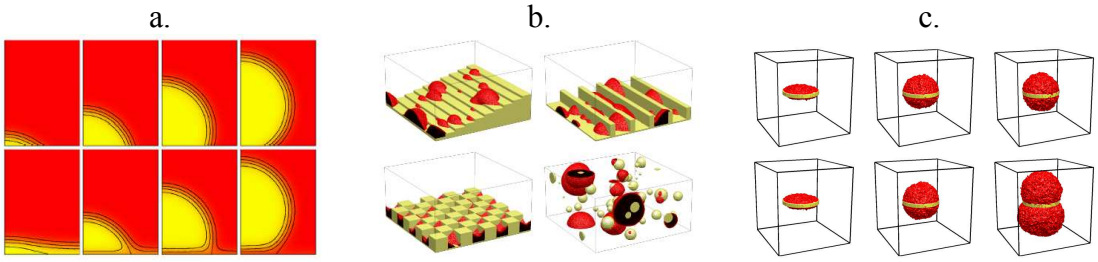

***Fig. 1**. Heterogeneous nucleation and inoculation in the PF model. (a) Structure of heterogeneous nuclei. Upper row – Model A: a diffuse interface version of the spherical cap model; bottom row – Model B: liquid ordering at the wall-liquid interface. (b) Heterogeneous nucleation on complex surfaces. (c) Inoculation of undercooled Ni by cylindrical particles of 20 nm diameter with contact angles of 45 ° and 175 ° on the horizontal and vertical surfaces. Upper row: $\Delta T = 26$ K $< \Delta T_c$, $t = 25, 250, 1000$ ns; bottom row: $\Delta T = 27$ K $> \Delta T_c$, $t = 25, 250, 750$ ns.*

The phase field theory has been applied to predict equilibrium interfacial properties and the nucleation barrier in the binary eutectic system Ag-Cu using double well and interpolation functions deduced from a Ginzburg-Landau expansion that considers fcc crystal symmetries. The model parameters are fixed so as to recover an interface thickness of ~1 nm from molecular dynamics simulations and the interfacial free energies from the experimental dihedral angles available for the pure components. Mapping the possible nucleation pathways, we find that the Ag and Cu rich critical fluctuations compete against each other in the neighborhood of the eutectic composition. The phase field predictions for the critical undercooling are found to be consistent with experimental results. We addressed crystal nucleation in the metastable liquid miscibility region of the eutectic system. It has been found that below the critical point, six different types of nuclei may

form: two liquid-liquid nuclei; two solid-liquid nuclei; and two types of composite nuclei, in which the crystalline core has a liquid "skirt", whose composition falls in between the compositions of the solid and the initial liquid phases, in addition to nuclei with concentric alternating composition shells of prohibitively high free energy.

We performed phase field simulations to estimate the conversion rate of CH_4 hydrate to CO_2 hydrate in the presence of liquid CO_2 under conditions typical for underwater gas hydrate reservoirs. In the computations, all model parameters are evaluated from physical properties taken from experiment or molecular dynamics simulations. We found that hydrate conversion is diffusion controlled, as after a short transient, the displacement of the conversion front scales with $t^{1/2}$. Assuming a diffusion coefficient of $D_s = 1.1 \times 10^{-11}$ m^2/s in the hydrate phase, the predicted time dependent conversion rate is in a reasonable agreement with results from Magnetic Resonance Imaging experiments. This value of the diffusion coefficient is higher than expected for the bulk hydrate phase, probably due to liquid inclusions remaining in the porous sample used in experiments.

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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 T 046700	Topochemical reactions in crystalline fullerenes and related materials (S. Pekker, 2004-2007)
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).

ESA PECS 98021 Phase field modeling of solidification in monotectic systems (T. Pusztai, 2005–2007)

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, IMPRESS Intermetallic Materials Processing in Relation to Earth and Space Solidification (T. Pusztai, 2004–2009)

OTKA K062588 Dynamics of complex systems (T. Pusztai, 2006-2009)

Alexander-von-Humboldt Foundation Joint Research Project 3-Fokoop-DEU/1009755, 2006-2008: 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)

EU FP6-STREP NMP4-CT-2006-031847, 2006-2009: "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)

EU FP6-Marie Curie Research Training Network MRTN-CT-2006-035810, 2006-2010: "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)

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)

Publications

Articles

E.1. Gránásy L, Pusztai T, Saylor* D, Warren* JA; Phase field theory of heterogeneous crystal nucleation; *Phys Rev Lett;* **98**, 035703/1-4, 2007

E.2. Tegze G, Gránásy L, Kvamme* B; Phase field modeling of CH_4 hydrate conversion into CO_2 hydrate in the presence of liquid CO_2; *Phys Chem Chem Phys;* **9**, 3107-3111, 2007

E.3. Tóth GI, Gránásy L; Phase field theory of interfaces and crystal nucleation in a eutectic system of fcc structure: I. Transitions in the one-phase liquid region; *J Chem Phys;* **127**, 074709/1-11, 2007

E.4. Tóth GI, Gránásy L; Phase field theory of interfaces and crystal nucleation in a eutectic system of fcc structure: II. Nucleation in the metastable liquid immiscibility region; *J Chem Phys;* **127**, 074710/1-8, 2007

E.5. Iwasiewicz-Wabnig* A, Sundqvist* B, Kováts É, Jalsovszky* I, Pekker S; Polymerization of the rotor-stator compound C60-cubane under pressure; *Phys Rev B*; **75**, 024114/1-10, 2007

E.6. Marković* Z, Todorović-Marković* B, Mohai* I, Farkas* Z, Kováts É, Szépvölgyi* J, Otašević* D, Scheier* P, Feil* S, Romčević* N; Comparative process analysis of fullerene production by the arc and the radio-frequency discharge methods; *J Nanosci Nanotechnol*; **7**, 1357–1369, 2007

E.7. Borondics F, Jakab* E, Pekker S; Functionalization of carbon nanotubes via dissolving metal reductions; *J Nanosci Nanotechnol*; **7**, 1551–1559, 2007

E.8. Iwasiewicz-Wabnig* A, Röding* R, Sundqvist* B, Kováts É, Jalsovszky* I, Pekker S; Pressure–temperature phase diagram of the rotor–stator compound C_{60}–cubane; *Solid State Commun*; **143**, 208–212, 2007

E.9. Klupp G, Kamarás K; Fulleride ions in various crystal fields studied by infrared spectroscopy; *J Mol Struct;* **838**, 74-77, 2007

E.10. Itkis ME*, Borondics F, Yu A*, Haddon RC*; Thermal conductivity measurements of semitransparent single-walled carbon nanotube films by a bolometric technique; *Nano Lett;* **7**, 900-904, 2007

E.11. Klupp G, Borondics F, Kováts É, Pekker Á, Bényei G*, Jalsovszky I*, Hackl R*, Pekker S, Kamarás K; Vibrational spectra of C_{60}•C_8H_8 and C_{70}•C_8H_8 in the rotor-stator and polymer phases; *J Phys Chem B;* **111**, 12375-12382*,* 2007

E.12. Faigel G, Bortel G, Fadley C*, Simionovici AS*, Tegze M; Ten years of x-ray holography; *X-ray Spectrometry*; **36**, 3-10, 2007

E.13. Bortel G, Faigel G; Classification of continuous diffraction patterns: a numerical study; *J Struct Biol*; **158**, 10-18, 2007

E.14. Oszlányi G., Sütő A.; Ab initio neutron crystallography by the charge flipping method; *Acta Cryst A;* **63**, 156-163, 2007

E.15. Vázsonyi É*, Dücső Cs*, Pekker Á; Characterization of the anisotropic etching of silicon in two-component alkaline solution; *J Micromech Microeng*; **17**, 1916-1922, 2007

Article in Hungarian

E.16. Pusztai T, Bortel G, Tóth G, Gránásy L; Komplex kristálymorfológiák modellezése három dimenzióban (3D modelling of complex crystal morphologies, in Hungarian); *Fizikai Szemle*; **56**, 412-415, 2006

Conference proceedings

E.17. Oszlányi G, Sütő A; The charge flipping method: a new approach to solve periodic and aperiodic structures; *Acta Cryst A;* **63**, s5, 2007, (invited lecture at the 24-th European Crystallographic Meeting, Marrakesh, Morocco, August 22-27 2007)

E.18. Tegze G, Gránásy L, Kvamme* B; Phase field modeling of the conversion of methane hydrate into carbon dioxide hydrate; In: *Proceedings of 4th WSEAS Int. Conf. on Heat and Mass Transfer, Gold Coast, Queensland, Australia, January 17-19*; pp. 27-29.

E.19. Faigel G, Bortel G,Tegze M; Hard x-ray holographic methods; In: *Proceedings of the NATO advanced research workshop on brilliant light in life and material sciences, Yerevan, Armenia, 17-21 July 2006*; Springer, ed. by V. Tsakanov and H. Wiedemann; pp. 383-393, 2007

F. LIQUID CRYSTALS

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

Synthesis. — *Banana shaped compounds* with a brand new architecture have been planned and synthesized. These compounds have a polymerizable double bond connected to position 5 of the central aromatic ring; we call this new family *bell-shaped* bananas. Though such compounds with symmetrical structure do not show liquid crystalline properties, they exhibit a melting point very close to room temperature. Therefore they are good candidates for being additives in liquid crystalline mixtures to obtain mesophases at, around and below room temperature.

The compounds with asymmetrical structure have required developing a more complicated synthetic procedure. These compounds with either a chiral or a fluorinated terminal group exhibited mesophases, which are now under investigation.

It has been shown that bent core (banana) compounds are miscible with some calamitic (rod like) nematics. A sequence of new mixtures has been prepared for flexoelectric investigations.

Electric field driven pattern formation. — Electric-field induced pattern forming instabilities (*electroconvection*, EC) of nematic liquid crystals have systematically been overviewed. The standard hydrodynamic description of nematics predicts the occurrence of striped patterns (rolls) in three basic configurations depending on the initial director orientation (planar or homeotropic) as well as on the anisotropy of the dielectric permittivity ε_a and that of the electrical conductivity σ_a. For planar aligned compounds with $\varepsilon_a < 0$, $\sigma_a > 0$ the EC pattern develops from an anisotropic basic state. At homeotropic boundary conditions the alignment has a rotational symmetry (isotropy in the cell plane) which is either broken spontaneously during a Freedericksz transition preceding the pattern forming instability (quasi-anisotropic case), or - at opposite sign of the anisotropies ($\varepsilon_a > 0$, $\sigma_a < 0$) - the isotropy is broken as part of the pattern forming mechanism. Experiments carried out for various initial geometries, like decay of patterns in planar, or magnetic field effects, abnormal rolls and defect dynamics in homeotropic cells, have shown excellent agreement with the theoretical predictions.

Though the standard model of electroconvection predicts no hydrodynamic instability for nematics with $\varepsilon_a < 0$, $\sigma_a < 0$, experiments have revealed convection patterns. This instability has been named as *non-standard electroconvection* (*ns-EC*). It has occurred in a bent core compound as well as in some nematics with an underlying smectic phase. We have characterized the *ns-EC* patterns in the latter compounds by measuring the frequency, thickness, and temperature dependence of the threshold voltage, the wave-number, and the roll orientation using polarizing microscopy or light diffraction, and compared them with the characteristics of the standard EC (*s-EC*). As in these compounds the conductivity anisotropy alters its sign on heating, a transition from *ns-EC* to *s-EC* could be induced by changing the temperature (Figure 1.a). We have also shown that at constant temperature a similar transition can be induced by the frequency or the applied voltage (Figure 1.b). For the first time, we have reported traveling rolls in *ns-EC*, and determined the dependence of the Hopf frequency on the temperature, the sample thickness and the driving frequency.

We have identified flexoelectricity as a possible source for the existence of the *ns-EC* patterns.

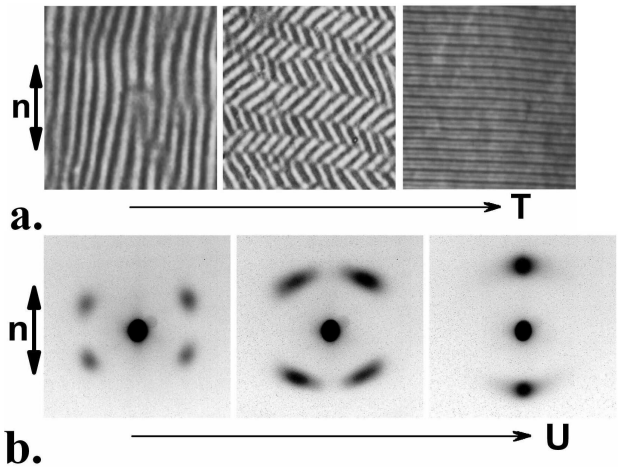

Fig. 1. *ns-EC to s-EC transition induced* ***(a)*** *by increase of the temperature T (polarizing microscopy);* ***(b)*** *by increase of the voltage U (light diffraction fringes).* ***n*** *denotes the initial director.*

Interactions at liquid crystal surfaces. — Experiments on *director gliding* have been carried out on Arabic gum and glucose layers. On Arabic gum flow alignment has been detected with permanent director orientation, while on glucose layers gliding has been found, which has speeded up above the glass-transition temperature of the glucose (32 ^{o}C). According to the first measurements, the distribution of relaxation times of the gliding process is much narrower for glucose than on corresponding polymer layers.

Granular flow. — The flow properties of a granular layer of thickness h on an inclined plane (inclination angle θ) can be characterized by the so called *flow rule*, which describes the thickness dependence of the surface velocity u. The flow rule of granular flows on a rough inclined plane has been measured for various materials, including sand and glass beads of various sizes and four types of copper particles with different shapes. The materials have been characterized by measuring h_s, the thickness at which the flow stops, as a function of the plane inclination on various surfaces. Measuring the surface velocity u of the gravity induced flow as a function of the flow thickness h, deviations from the Pouliquen flow rule $u/(gh)^{0.5} \sim h/h_s$ have been detected for sand and glass beads. An improved collapse of the experimental data has been obtained by using a recently proposed scaling of the form $u/(gh)^{0.5} = \beta\, h\tan^2\theta / h_s \tan^2\theta_1$ where θ_1 is the angle at which the h_s curves diverge. Measuring the slope β for ten different sizes of sand and glass beads, we find a systematic, strong increase of β with the divergence angle θ_1. Copper materials with different shapes could not well be described by either flow rule.

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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)

63ÖU4 (Hungarian Action Foundation) Advanced liquid crystals with unique architecture (K. Fodor-Csorba, 2006-2007)

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

MTA-WATWAW (Hungarian–Polish bilateral) Study of liquid crystals (K. Fodor-Csorba, 2005-2007)

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)

Long term visitors

— Michal Kohout: Institute of Chemical Technology, Prague, Czech Republic, 1 April - 31 May, 2007 (COST D35 WG 13/05, host: Fodor-Csorba K)

— Yoshio Shimbo: Tokyo Institute of Technology, Tokyo, Japan, 3 July - 13 August, 2007 (MTA-JSPS, host: Éber N)

— Prof. Antal Jákli: Liquid Crystal Institute, Kent State University, Kent, USA, 9 July - 13 August, 2007 (host: Éber N)

— Anel Flores Amado: Centre de Investigation en Polimeros, Mexico, 20 May – 20 June, 2007 (MTA-CONACYT, host: Fodor-Csorba K)

— Jana Heuer: Otto von Guericke University, Magdeburg, Germany, 1 – 30 November, 2007 (host: Buka Á)

Publications

Articles

F.1. Börzsönyi T, Ecke* R E; Rapid granular flows on a rough incline: phase diagram, gas transition, and effects of air drag; *Phys Rev E*; **74**, 061301/1-9, 2006

F.2. Domenici* V, Fodor-Csorba K, Frezzato* D, Moro* G, Veracini* C A; Deuterium NMR evidences of slow dynamics in the nematic phase of a banana-shaped liquid crystal; *Ferroelectrics*; **344**, 19-28, 2006

F.3. Sovic* T, Kappaun* S, Koppitz* A, Zojer* E, Saf* R, Bartl* K, Fodor-Csorba K, Vajda A, Diele* S, Plezl* G, Slugovc* C, Stelzer* F; Main-chain Liquid Crystalline Polymers Based on Bis-etherified 9,9-dihexyl-2,7-bis(4'-hydroxy-1,1'-biphen-4-yl)fluorenes; *Macromol Chem Phys;* **208**, 1458-1468, 2007

F.4. Calucci* L, Forte* C, Fodor-Csorba K, Mennucci* B, Pizzanelli* S; Conformations of banana–shaped molecules studied by ^{2}H NMR spectroscopy in liquid crystalline solvents; *J Phys Chem B;* **111**, 53-61, 2007

F.5. Domenici* V, Veracini* CA, Fodor-Csorba K, Prampolini* G, Cacelli* I, Lebar* A, Zalar* B; Banana-shaped molecules peculiar orientated in a magnetic field: ^{2}H NMR spectroscopy and quantum mechanical calculations; *Chem Phys Chem;* **8**, 2321-2330, 2007

F.6. Tóth-Katona T, Cauquil-Vergnes* A, Éber N, Buka Á; Non-standard electroconvection with Hopf-bifurcation in a nematic with negative electric anisotropies; *Phys Rev E;* **75**, 066210/1-12, 2007

F.7. Börzsönyi T, Ecke* RE; Flow rule of dense granular flows down a rough incline; *Phys Rev E;* **76**, 031301/1-10, 2007

F.8. Buka Á, Éber N, Pesch* W, Kramer* L; Isotropic and anisotropic electroconvection; *Phys Reports;* **448**, 115-132, 2007

F.9. Jánossy I, Vajda A, Statman* D; Influence of the molecular weight of a polymer on the gliding of nematic liquid crystals; *Mol Cryst Liq Cryst;* **466**, 77-82, 2007

F.10. Bubnov* A, Hamplova* V, Kaspar* M, Vajda A, Garic* M, Obadovic* DZ, Éber N, Fodor-Csorba K; Thermal analysis of binary liquid crystalline mixtures: system of bent core and calamitic molecules; *J Therm Anal and Cal;* **90,** 431-441, 2007

F.11. Krekhov* A, Pesch* W, Éber N, Tóth-Katona T, Buka Á; Nonstandard electroconvection and flexoelectricity in nematic liquid crystals; *electronic-Liquid Crystals Communications;* http://www.e-lc.org/docs/2007_09_14_08_02_35, 2007

F.12. Statman* D , Basore* V, Sulai* Y, Dunlap* B, Jánossy I; Photoinduced gliding of the surface director in azo-dye doped nematic liquid crystals; *Liq Cryst*; accepted for publication.

Article in Hungarian

F.13. Börzsönyi T; Lejtőn lefolyó szemcsés anyag dinamikája: instabilitások, lavinák (Dynamics of granular materials on an inclined plane: instabilities, avalanches, in Hungarian); *Fizikai Szemle*; LVII(7), 217-220, 2007.

Conference proceeding

F.14. Éber N, Jákli A*, Harden* J , Gleeson* JT, Wiant* D, Sprunt* S, Fodor-Csorba K, Tóth-Katona T, Buka Á; Flexoelectricity and electroconvection in a banana nematic; In: *Proceedings of International Conference on Liquid Crystals*; Mumbai, India, 2006, accepted for publication.

G. ELECTRON CRYSTALS

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

Dissipation in high-T_c superconductors. — Most high-magnetic-field applications of superconductors are limited by dissipative mechanisms. To investigate this important problem, we have collected and analyzed a large body of data on the dissipation at high transport currents in single crystals of the cuprate superconductor $Bi_2Sr_2Ca_2CuO_8$. We have found that several aspects of the dissipative processes are in disagreement with the current theoretical understanding of this important model system of high-temperature superconductors. We have discovered a new scaling law of the resistance valid sufficiently close to the critical temperature where the superconductivity sets on. According to this law, the resistance depends on temperature only through the upper critical magnetic field H_{c2}, one of the fundamental parameters of the superconductor related to the size of Cooper pairs. Moreover, the resistance varies logarithmically with magnetic field, rather than following a power law as in conventional superconductors. Nevertheless by a re-analysis of experimental results in the literature, we have shown that for transport currents flowing parallel to the superconducting planes of this layered material, a power law is still valid, although the exponent ¾ is different from that described by the well known Bardeen-Stephen law for conventional superconductors. We have also found an analytic form for the resistance perpendicular to the superconducting layers, which is in good agreement with experimental results.

Microwave Spectroscopy. — Two-dimensional systems, be they electrons, holes or superconducting vortices, lend themselves well to investigation by finite-wavevector near-field microwave spectroscopy. It is planned to study holes at GaAs/GaAlAs heterojunctions in the Wigner solid phase, electrons/holes in graphene in the quantum Hall regime and Kelvin modes of quasi 2-D vortices in BSCCO ($Bi_2Sr_2CaCu_2O_8$, an extremely anisotropic high temperature superconductor). To this end we have prepared a 0.1-10 GHz swept-frequency low-level source and low noise (noise temperature ~200K) superheterodyne detector which will be used with our 30 mK dilution refrigerator in the mixing chamber of which is a microstrip meander line coupling device connected through low thermal loss, high-transmittance Cu-Kapton based transmission lines. This alone enables us to do microwave spectroscopy up to wavevectors of ~ 10^5 cm^{-1}, but with the adjunction of a nanolithography-manufactured grid of 300 nm periodicity the range should be extended to ~ 10^6 cm^{-1}. The refrigerator has been designed to be placed in high magnetic field (28 T) at the Grenoble high magnetic field facility when necessary; otherwise it is run in our local 8 T coil.

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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 Condense (SPEC) CEA-Saclay, France on electron crystals and nano-electronics (2005-2008)

Publications

Articles

G.1 Matus P, Alloul* H, Kriza G, Brouet* V, Singer* PM; S. Garaj* S; Forró* L; Influence of local fullerene orientation on the electronic properties of Na_2AC_{60} (A = Cs,Rb,K) compounds; *Phys Rev B;* **74**, 214509/1-11, 2006

G.2 Matus P, Alloul* H, Kriza G, Brouet* V, Singer* PM, Garaj* S, Forro* L; NMR evidence for C-60 configurational fluctuations around Na sites in Na_2CsC_{60}; *J Supercond Nov Magn* **20**, 155-159, 2007

See also:

H. METAL PHYSICS

K. Tompa, I. Bakonyi, P. Bánki, M. Bokor, Cs. Hargitai, Gy. Lasanda, L. Péter, E. Tóth-Kádár

Metal-hydrogen systems. — We have in-situ investigated hydrogen charging (discharging) processes in $Pd_xAg_{1-x}H$ alloys by simultaneous hydrogen concentration and nuclear spin-spin relaxation time measurements.

Hydration of intrinsically disordered proteins. — ^{1}H NMR signals of physiological solutions of proteins were investigated (in cooperation with the Institute of Enzymology, Biological Research Center, HAS). The principal aim of our work is to characterize structural and dynamical properties of interfacial water at the protein surface by wide-line NMR spectroscopy and nuclear relaxation time measurements for the identification and characterization of intrinsically disordered proteins (IDPs) and to make a distinction between IDPs and globular proteins. Our approach is to explore the structure↔interface relations of IDPs and globular proteins. The main results are the direct determination of the number of hydration water molecules, the elements of hydration water dynamics (activation energy and correlation times), and the differences in dynamics as seen by the different time windows provided by the different types of relaxation rates (R_1, $R_{1\rho}$ and R_2). We have shown by several examples that IDPs (e.g. early responsive to dehydration 10, caskin, histone chaperone Df31) are distinguished from globular proteins (e.g. bovine serum albumin, ubiquitin) by their more extended interfacial region (hydration), the stronger (spin diffusion- and chemical-) interactions between protein and bound water at low temperatures and the higher relaxation rates and activation energies at high temperatures. Proteins dissolved in distilled water are surrounded by a homogeneous hydrate shell while in buffered solvent the hydrate shell is more complex and involves more water molecules (Fig. 1). From the combined analysis of the DSC traces and the amount of hydration water measured by NMR, we have determined the specific heat of the system consisting of the protein molecule and its hydration shell. The NMR investigations have been extended to lyophilized (solid state) protein samples (Fig. 2) to get structural information on the protein molecules e.g. motional states of methyl and methylene groups.

Electrodeposition. — Electrochemical deposition of Pd-Cu alloys was investigated by using voltammetric methods and an electrochemical quartz crystal microbalance (EQCM). It was found that deposit composition changes continuously with electrode potential. The codeposition of Cu was observed also in the potential range where Cu cannot be deposited alone, but Cu underpotential deposition onto Pd can take place. Hence, the process of the Pd-Cu codeposition is an accumulative underpotential deposition. The deposit weight calculated from the frequency change of the quartz crystal microbalance during potential sweeps is in good agreement with the elemental analysis performed on samples produced by ex-situ potentiostatic deposition.

A new operation mode was elaborated with a potentiostat and the EQCM. While formerly the microbalance has always been used as an additional detector of the surface weight change, in our workstation it can now be used as a part of the regulation. This so-called feedback mode enabled us to modify the deposition conditions in-situ and to deposit alloys with either stabilized composition or with a predefined depth profile. The system was tested successfully for the deposition of Pd-Cu alloys.

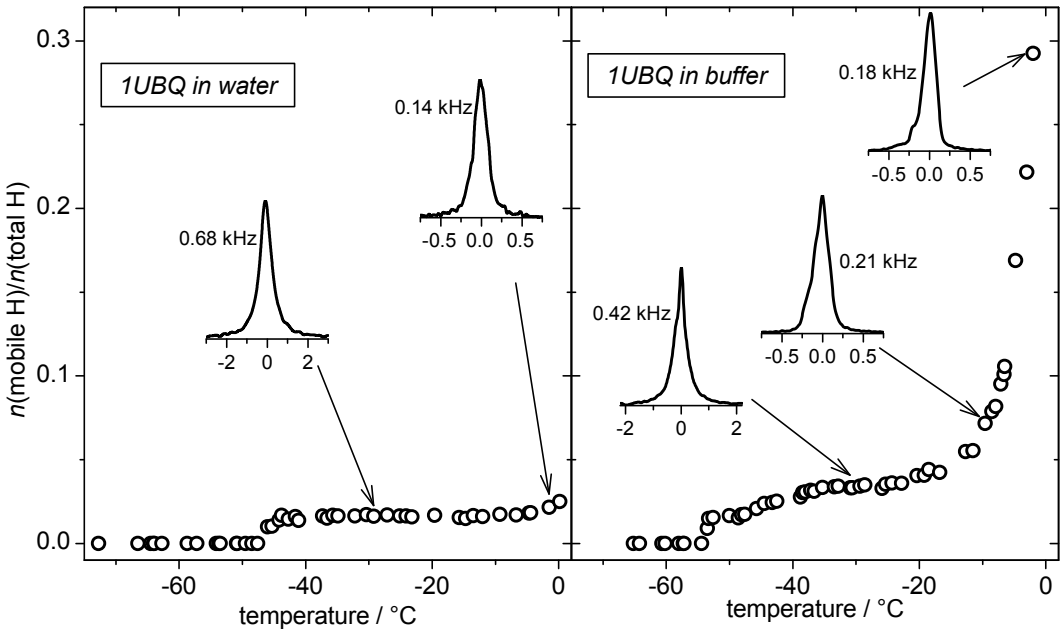

Fig. 1. *^{1}H NMR spectra and mobile water fractions x = n(mobile H)/n(total H) determined from ^{1}H-NMR signal intensities for 41 mg/cm^3 ubiquitin dissolved in water (left graph) and in buffer (right graph). Spectra (inserted graphs) are Fourier-transformed FID signals on frequency scale in kHz units. Full widths at half maxima (fwhm) are given for each spectrum. The concentrations of mobile ^{1}H nuclei (circles) correspond to water molecules in a mobile motional state. The width (fwhm) of the spectra above 0 °C can be taken as a measure of the inhomogeneity of the applied static magnetic field B_0; it is 0.14 kHz for the pure water solution (left graph) and it is 0.19 kHz for the buffered solution (right graph). At low temperatures where the water content is completely frozen, the fwhms of the spectra are on the scale of 10 kHz for both solvents.*

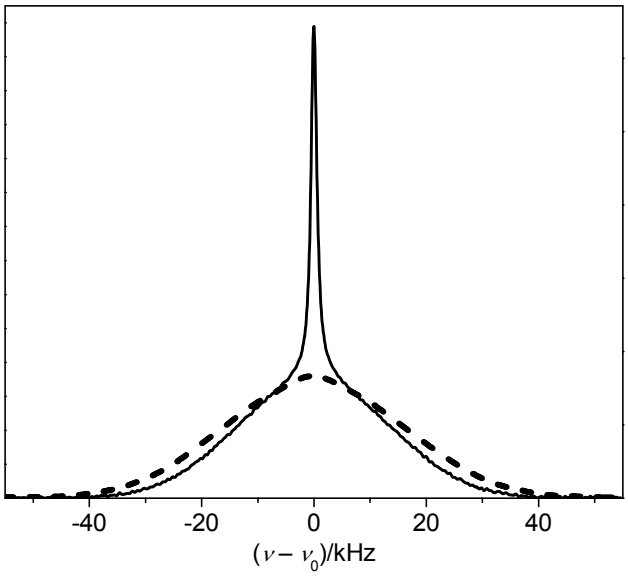

Fig. 2. *^{1}H-NMR spectra for lyophilised ubiquitin at +24.8 °C (solid line) and at -74.5 °C (dashed line). The origin of the narrow component at high temperature is the water content of the sample (12.7 wt%). The broad component originates from protons of the ubiquitin molecule.*

Structure and GMR of electrodeposited multilayers. — The room-temperature magnetoresistance (MR) of electrodeposited Co-Cu/Cu multilayers was investigated. Samples were prepared on either a polycrystalline Ti foil or on a silicon wafer covered with a Ta buffer and a Cu seed layer. Along the lines of our recent works, the field-dependence of the magnetoresistance was analyzed by decomposing the GMR into ferromagnetic (FM) and superparamagnetic (SPM) contributions, whereby the field-dependence of the latter could be described by a Langevin function. It has been shown that the non-monotonic change in the saturation field and in the full width at half-maximum of the magnetoresistance curves of Co-Cu/Cu multilayers as a function of the Cu layer

thickness can be elucidated by decomposing the full magnetoresistance curves into FM and SPM contributions. The decomposition analysis revealed that a minimum observed in the total magnetoresistance is caused by an interplay between the monotonously decreasing SPM contribution and the monotonously increasing FM contribution (Fig. 3). Both components achieved a saturation value at $d_{Cu} > 3.2$ nm. The variation of the FM and SPM contributions can be successfully explained by the island model of the SPM regions. While the SPM cluster size is independent of d_{Cu}, the peak position of the MR curves is higher when the magnetoresistance components achieved their saturation value. This is consistent with the assumption that the saturation is related to the more complete separation of the magnetic layers as d_{Cu} increases. A comparison of the multilayer series deposited onto Ti and Si/Ta/Cu substrates revealed that the lower surface roughness of the latter substrate leads to a reduced SPM contribution and, hence, to a higher magnetoresistance sensitivity close to zero field. The reduced SPM contribution of samples obtained with smooth Si/Ta/Cu substrates is a consequence of the structural improvement of the multilayers.

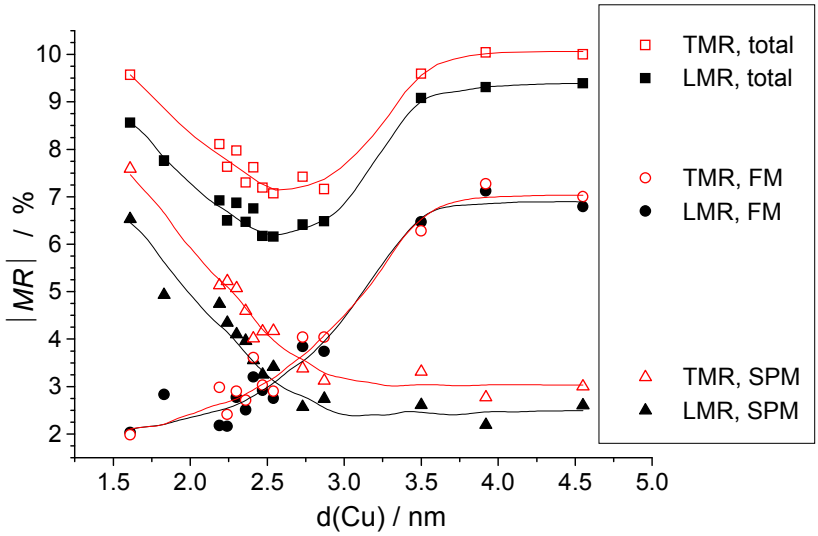

Fig. 3 *Evolution of the total (saturation) magnetoresistance and the FM and SPM contributions with Cu layer thickness for a multilayer series electrodeposited on Ti. The magnetic layer thickness was 2.0 nm. Lines are intended only as a guide for the eye.*

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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)

Wellcome Trust ISRF GR067595MA Study of partially structured protein solutions (2005-2007). The RISSPO is subcontractor (project leader: K. Tompa) in this research grant for the Institute of Enzimology of HAS.

TéT RO-22/05 Hungarian-Romanian Bilateral Collaboration: GMR mulitlayer structures (I. Bakonyi, 2006-2007)

Publications

Articles

H.1. Katona* GL, Berényi* Z, Péter L, Vad* K; Depth profile analysis of electrodeposited nanoscale multilayers by SNMS; *Vacuum* **82**, 270-273, 2007

H.2. Mankovsky* S, Bakonyi I, Ebert* H; Magnetic susceptibility contributions and electronic density of states in $(Ti,Zr)_{100-x}(Ni,Cu)_x$ metallic glasses and crystalline compounds; *Phys Rev B*; **76**, 184405/1-15, 2007

H.3. Péter L, Pádár J, Tóth-Kádár E, Cziráki* Á, Sóki* P, Pogány L, Bakonyi I; Electrodeposition of Co-Ni-Cu/Cu multilayers 1. Composition, structure and magnetotransport properties; *Electrochim Acta*; **52**, 3813-3821, 2007

H.4. Péter L, Katona* GL, Berényi* Z, Vad* K, Langer* GA, Tóth-Kádár E, Pádár J, Pogány L, Bakonyi I; Electrodeposition of Ni-Co-Cu/Cu multilayers 2. Calculations of the element distribution and experimental depth profile analysis; *Electrochim Acta*; **53**, 837-845, 2007

H.5. Péter L, Weihnacht* V, Tóth J, Pádár J, Pogány L, Schneider* CM, Bakonyi I; Influence of superparamagnetic regions on the giant magnetoresistance of electrodeposited Co-Cu/Cu multilayers; *J Magn Magn Mater;* **312**, 258-265, 2007

H.6. 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;* (accepted for publication)

H.7. 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;* accepted for publication

Book chapters

H.8. Szalma* J, Láng* Gy, Péter L; Alapvető fizikai-kémiai mérések és a kísérleti adatok feldolgozása (Basic physical chemistry measurements and evaluation of experimental data, in Hungarian); ELTE Eötvös Kiadó, Budapest, pp. 1-211, 2007

H.9. Tompa K, Bokor M, Tompa* P; Chapter 10. Hydration of intrinsically disordered proteins from wide-line NMR; In: *Assessing Structures and Conformations of Intrinsically Disordered Proteins;* Eds.: Uversky V.N. and Longhi S, Nova Science Publishers, New York; accepted for publication

See also: D.12., I.3.

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 (GFA) of Cu-based alloys have been studied in collaboration with the Materials Science Department of Miskolc University, Hungary. Several compositions have been prepared, following the bulk GFA criteria published so far in the literature, such as $Cu_{100-x-y-z}Zr_xTi_yAg_z$, Cu_{100-x} Mm_xAl_y where Mm means Mischmetal.

Surveying all the Cu-based amorphous alloys published in the literature so far, it turned out that the atomic mismatch condition of Egami and Waseda is fulfilled for all the Cu-based bulk amorphous alloys, the λ value being above 0,3. Combining the chemical coordinates of Miedema (y) with the atomic mismatch (x), the glass forming and non-glass forming regions were found separated by the following curve: $y=|10|\Delta\Phi^*|-39\ |\Delta(1/n_{ws}^{1/3}|-1|$ and $x=|1-R_x/R_{Cu}|$ for the binary Cu-based alloys.

The glass forming ability of Al-based alloys (mainly of $Al_{85}Mm_5Ni_8Co_2$ type compositions) has been investigated during the compaction of powders obtained by gas atomising and chopping the rapidly quenched ribbons.

Soft magnetic nanocrystalline alloys. — Based on a Quasi-DC hysterograph, an experimental technique has been developed to obtain the true "static" hysteresis curve. This is the so-called "ballistic "method to obtain the hysteresis loop by integrating the measured incremental permeability ($\mu_{incremental} = \mu_{diff}$) versus biasing DC field, H_{DC}. In addition, it was demonstrated that it is possible to decompose the quasi-static hysteresis loop into two contributions deriving from domain magnetization rotation (DR) and domain wall movement (DWM) (Fig. 1 and Fig. 2) and this decompositon was modelled theoretically by the hyperbolic T model. The hyperbolic T model was further improved by splitting it in 3 overlapping hysteretic contributions: one DR and two DWM (jumping and annihilation) parts. Softwares have been developed to carry out measurements of reversible magnetization at very small excitation ($H_{\sim}$ <<Hc) and at fixed frequencies between 100 and 20000 Hz.

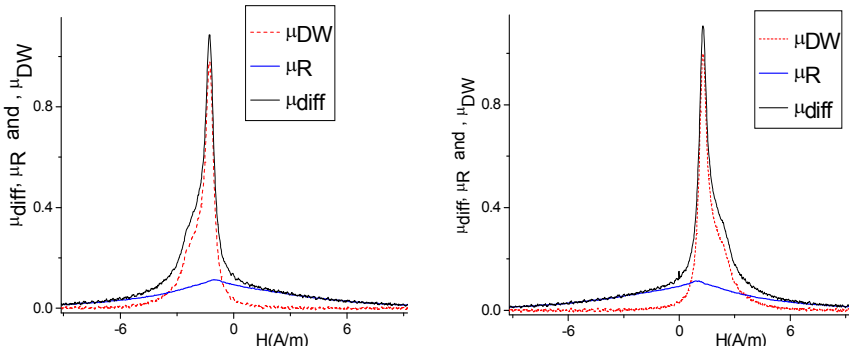

Fig. 1. *The measured μ_{diff} and μ_R and the calculated $\mu_{DW} = \mu_{diff} - \mu_R$ as a function of the biasing DC field for descending (a) and ascending branches (b), respectively.*

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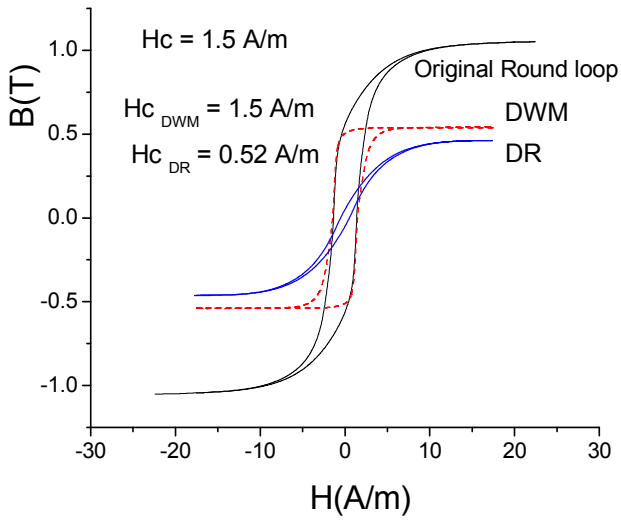

Fig. 2. *The measured original major loop and the experimentaly decomposed (DWM, DR) loops.*

Thermal, thermomagnetic and thermomechanical testing of amorphous alloys. – Fe-based metallic glasses are interesting materials from the point of view of their excellent soft magnetic properties. However, recently they have attracted attention due to their superior mechanical properties as well such as the thermoplastic behavior compared with ordinary metals observed in the temperature region of the glass transition. Materials with combined properties of metals and polymers have potential in applications everywhere where polymeric plastics are not applicable (e.g. high temperature, high mechanical stress).

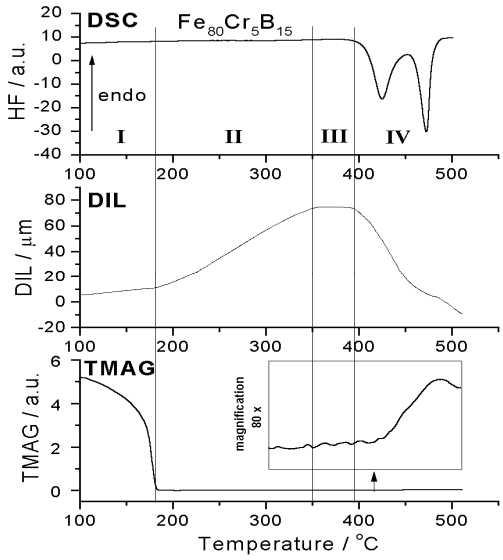

Fig. 3. *Experimental data on thermal (DSC), dilatometric (DIL), and thermomagnetic (TMAG) behavior of an amorphous $Fe_{80}Cr_5B_{15}$ alloy in the temperature range up to crystallization, which can be divided into four regions: I- ferromagnetic amorphous alloy up to Curie point, II – paramagnetic amorphous alloy, III – softening associated with glass transition recorded by DIL, IV – primary and secondary crystallization revealed by DSC. Recreated magnetization recorded by TMAG indicates a new ferromagnetic phase formed in this region. Heating rate: 20 K min^{-1}.*

In order to get more comprehensive information about the observed phenomenon, three experimental methods were applied: alternating current thermomagnetometry (TMAG), differential scanning calorimetry (DSC) and temperature modulated dilatometry (TM DIL). The latter experiment was developed in cooperation with the Technical University of Koszalin, Poland. The method allows obtaining thermal expansion coefficient of ribbon-shaped samples under very low tracking force. The modulation added to the

temperature profile increases the sensitivity by about two orders of magnitude and allows the separation of reversible and irreversible processes.

The methods have been used to investigate transformations of amorphous alloys before crystallization. Results obtained for $Fe_{80}Cr_5B_{15}$ are depicted in Fig 3. There are visible changes in mechanical behavior of the material (trace DIL) associated with magnetic and structural transitions.

The mentioned methods together with the newly developed high heating-rate differential thermal analysis (DTA) (see Annual Report 2006), allow to get comprehensive information about kinetics of the devitrification processes. Methods are applied in the research program on metastable alloys as multicomponents bulk alloys, in collaboration with the Technical University of Koszalin and Budapest University of Technology and Economics. Dilatometric measurement with DSC is promising in the investigation of Al-based bulk amorphous alloys that are produced in our institute.

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Grants and international cooperations

OTKA K62466	Investigation of the deterioration of power plant construction materials by magnetic methods (Project leader: J. Ginsztler (BME), SZFKI participant: L.K. Varga, 2006-2009)
HAS-BAS	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, Hungarian-Bulgarian Academy Exchange Programme)
HAS-SAS	Study of physical properties of special magnetic materials (L.K. Varga, 2005-2007, Hungarian-Slovakian Academy Exchange Programme)
HAS-PAS	Investigation of thermophysical properties of coatings (P. Kamasa, 2005-2007, Hungarian-Polish Academy Exchange Programme)
TOMMY-INVEST	ELECTRONICS LTD. Development of magnetic field annealing for the inductive electronic component market (Project leader: L.K. Varga)
SEM analysis	Failure analysis of various mechanical and electronic components for the industry by SEM (Project leader: L. Pogany)

Publications

Articles

I.1 Mikó* A, Kuzmann* E, Lakatos-Varsányi* M, Kákay A, Nagy* F, Varga LK; Mössbauer and XRD study of pulse-plated Fe-P and Fe-Ni thin layers; *Hyperf Int*; **165**, 195-201, 2005

I.2 Fazakas E, Varga LK, Mazaleyrat* F; Preparation of nanocrystalline Mn-Al-C magnets by melt spinning and subsequent heat treatments; *J All Comp*; **434-435**, 611-613, 2007

I.3 Kamasa P, Bokor M, Pyda* M, Tompa K; DSC approach for the investigation of mobile water fractions in aqueous solutions of NaCl and Tris buffer; *Thermochim Acta* **464**, 29-34, 2007

I.4 Kane* SN, Gercsi Zs, Mazaleyrat* F, Rodionov* D, Bernhardt* B, Klingelhöfer* G; Surface analysis of Fe-Co-Nb-Cu-B metallic glasses using a miniaturised Mössbauer spectrometer 'MIMOS'; *J Non-Cryst Sol;* **353**, 3587-3589, 2007

I.5 Kane* SN, Gercsi Zs, Mazaleyrat* F, Varga LK, Gupta* A, Coisson* M, Tiberto* P, Vinai* F, Celegato* F; Influence of annealing on the high frequency magnetotransport properties of melt-spun $Fe_{31}Co_{31}Nb_8B_{30}$ alloys; *J Non-Cryst Sol;* **353**, 3099-3102, 2007

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I.7 Mikó* A, Takács* M, Lakatos-Varsányi* M, Varga LK; Pulse plated amorphous Fe-P thin layers for high frequency magnetic applications; *Mater Sci Forum*; **537-538**, 231-237, 2007

I.8 Myslinski* P, Kamasa P, Gilewicz* A, Staskiewicz* J: Detection of mechanical effects of adhesive thin films on substrate using the modulated-temperature dilatometry (MT DIL); *J Therm Anal Calorim* **88**, 737-740, 2007

I.9 Varga LK; Soft magnetic nanocomposites for high frequency and high temperature applications; *J Magn Magn Mater*; **316**, 442-447, 2007

I.10 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;* accepted for publication

I.11 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;* accepted for publication

I.12 Kane* SN, Gercsi* Zs, Mazaleyrat* F, Varga LK, Coisson* M, Tiberto* P, Vinai* F, Celegato* F, Jeong* YH; Influence of composition and thermal treatments on structural, magnetic and magnetotransport properties of $(Fe_{100-x}Co_x)_{78}Si_9Nb_3B_9Cu_1$ alloys; *J Korean Phys Soc;* accepted for publication

I.13 Kane* SN, Khinchi* SS, Gercsi* Zs, Gupta* A,Varga LK, Mazaleyrat* F, Jeong* YH; Structural and magnetic investigation of amorphous and gradually devitrified nanocrystalline Fe-Co-Nb-Cu-B alloys; *J Korean Phys Soc;* accepted for publication

I.14 Varga LK, Kovács* Gy; Separation of magnetization loop in domain wall movement and domain rotation contributions for soft magnetic materials; *Acta Physica Polonica A;* accepted for publication

I.15 Varga LK, Kovács* Gy, Takács* J; Modeling the overlapping, simultaneous magnetization processes in ultrasoft nanocrystalline alloys; *J Magn Magn Mater*; accepted for publication

Conference proceedings

I.16 Kuzmann* E, Lakatos-Varsányi* M, Varga LK, Mikó* A, Kálmán* E, Homonnay* Z, Nagy* F, Vértes* A; Mössbauer study of electrodeposited Fe/Fe-oxide multilayers; *AIP Conf. Proc.* **765**, 211–216, 2005

Other

I.17 Bárdos* A, Stoica* M, Varga LK, Roth* S, Schultz* L; Verfahren zur Herstellung metalhaltiger Gusskörper und Vorrichtung dafür, (Process and equipment for the preparation of metal-containing ingots, in German); *German Patent* DE 10 2005 037 982 B3 2007.03.15

See also: H.3., H.4., H.5.

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, G. Pépy, E. Rétfalvi[#], Zs. Sánta[#], N.K. Székely[#], Gy. Török, T. Veres[#]

Structure of soft condensed matter – aqueous solutions. The structure and properties of aqueous tetramethylurea (TMU) solutions, as well as the intermolecular interactions in their solutions, were widely studied by different experimental and theoretical techniques. The special interest is attributed to the mainly hydrophobic character of the hydration due to the four methyl groups on the nitrogen atoms. Our previous studies indicated significant hydrophobic interaction between TMU molecules which becomes more attractive at higher temperatures. We extended our study to some TMU derivatives. Small angle neutron scattering (SANS) studies of the solutions of N,N-dimethylelthyleneurea (DMEU) in heavy water (D_2O) and N,N-dimethylpropyleneurea (DMPU) in D_2O were carried out as a function of concentration and temperature. The DMEU represents the cyclic analogue of TMU, it contains instead of two methyl groups an ethylene group, and thus has a ring structure. The DMPU is the homologue of DMEU, it has a propylene group in the ring, instead of an ethylene group. Comparing the results obtained for the solutions of DMEU and DMPU with those previously reported for TMU conclusions can be drawn about how the structural differences between these molecules affect the intermolecular interactions. Following the temperature and concentration dependence of the second osmotic virial coefficient (B/Vp) calculated from SANS results, the character of the interactions between the solute molecules can be estimated. If the values of B/Vp are more and more negative with increasing temperature, the pair interaction between the molecules becomes stronger. The hydrophobic interaction is stronger at higher temperatures. We compared the B/Vp values obtained for DMEU and DMPU solutions with those for TMU (Fig.1). In sharp contrast with the values for TMU solutions, the second osmotic virial coefficients of DMEU and DMPU are constant (within the experimental precision) with increasing temperature. Such behavior may suggest that the attractive DMEU-DMEU, and DMPU-DMPU interactions, in their aqueous solutions, is not of the hydrophobic type.

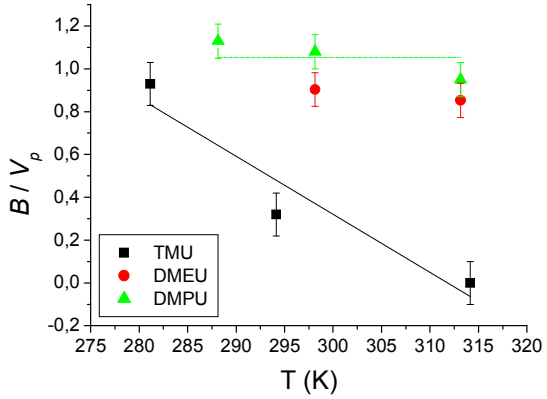

Fig. 1. *Temperature dependence of the dimensionless second osmotic virial coefficient (*B/Vp*) for the solutions of TMU, DMEU and DMPU in D_2O.*

Applied research with neutrons – irradiation damage of reactor components. Damaged control rods of the WWR-M10 Budapest research reactor were measured by

[#] Ph.D. student

SANS. The measured 3 control rods were: K1 (ZfK VA58), K5 (ZfK VA53), Non-used (ZfK VA77). The characteristics were as follows. Chemical composition: AlMgSi (Mg(0.9), Si(0.7), Cu(0.1), Mn(0.1), Fe(0.4), Zn(0.2), Ti(0.2) % in Al matrix) rod filled with B_4C powder. Size: the diameter is 27mm and the total length is 786mm. Preparation: pulling and homogenization on high temperature (550 °C). Gamma activity: on surface (measurement time June of 2005) K5 : 26mSv/h, K1:260mSv/h. We have measured 19 points along the rod. The distance between the measured points is 20mm. We turned the rod with 90° to measure all side of the rod. The rod was covered with thin Al foil to avoid the measuring place from the possible radioactive fall out.

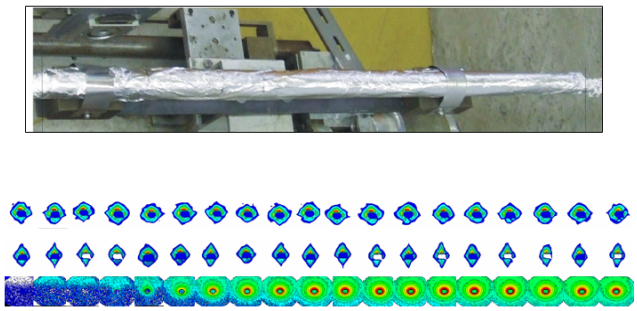

Fig. 1.

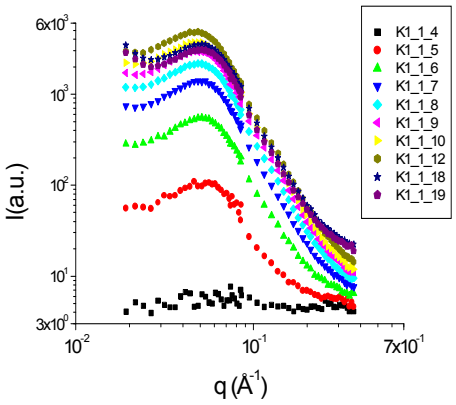

Fig. 2.

Fig. 1 shows the rod on the sample stage of the SANS instrument, SANS spectra recorded alongside the rod and the integrated intensity distribution as a function of the momentum transfer for the different positions of the rod are given in Fig. 2. A clear correlation of the irradiation damage (the SANS curves reveal the pore structure evolution in the alloy material) is followed along the rod as a function of the flux distribution in the height of the reactor core.

Neutron instrumentation. The 10 MW Budapest Research Rector (BRR) and its experimental facilities on the KFKI site is a unique large-scale facility in the Central European region. The Neutron Spectroscopy Department is one of the Laboratories of the associate institutes forming the Budapest Neutron Centre, which is open for the domestic and international user community and serves for basic and applied research, commercial utilisation and education. Experiments performed by the local staff and in collaboration with national or foreign users coming from universities, industrial or other research laboratories. We operate several cold and thermal neutron beam instruments: a small angle scattering (SANS) spectrometer, a reflectometer (REFL), a three axis spectrometer (TASC) and a cold neutron beam test facility as well as a thermal beam three axis spectrometer (TAST) and time-of-flight diffractometer (TOFD).

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Grants and international cooperations

EU HII3-CT-2003-505925 Access to Research Infrastructure (BNC, L. Rosta, 2004-2007)

EU HII3-CT-2003-505925 Access to Research Infrastructure (BNC, L. Rosta, 2004-2007)

EU HII3-CT-2003-505925 JRA2 Detector Development project (L. Rosta, 2004-2007)

EU HII3-CT-2003-505925 JRA3 Focusing Neutron Optics project (J. Füzi, 2004-2007)

EU HII3-CT-2003-505925 JRA2 Polarised Neutron Techniques (Gy.Török, 2004-2007)

IAEA-13507 Improvement of Neutron beam performance and sample environment in residual stress (Gy. Török, 2006-2007)

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)

TET CZE- 2005 Solutions (L. Almásy, 2005-2007)

Study of nanostructures in functional materials by means of neutron scattering at the Frank Laboratory of Neutron Physics (FLNP) of the Joint Institute for Nuclear Research (JINR), Dubna (L.Rosta, 2005- 2007.)

Introduction of young scientists and researches working at the BNC into the use of time-of-flight method realized by the experimental trainings and courses at the IBR-2 Pulsed Reactor at the Frank Laboratory of Neutron Physics (FLNP) of the Joint Institute for Nuclear Research (JINR), Dubna (L.Rosta, 2006 - 2007.)

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Articles

J.1. Cser L, Török Gy, Krexner* G, Markó M, Sharkov* I; Direct observation of local distortion of crystal lattice with picometer accuracy using atomic resolution neutron holography; *Phy Rev Letters;* **97**, 255501/1-4, 2006

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J.3. Avdeev* MV, Tropin* TV, Aksenov* VL, Rosta L, Garamus* VM, Rozhkova* NN; Pore structures in shungites as revealed by small-angle neutron scattering; *Carbon*; **44,** 954–961, 2006

J.4. Aksenov* VL, Avdeev* MV, Kyzyma* OA, Rosta L, Korobov* MV; Age effect of solution C_{60}/N-methilpyrrolidone on the cluster structure in the system C_{60}/N-methilpyrrolidone/water; *Crystallography reports;* **52,** 523-527, 2007

J.5. Almásy L, Len A, Székely NK, Plestil* J; Solute aggregation in dilute aqueous solutions of tetramethylurea; *Fluid Phase Equilibria;* **257,** 114-119, 2007

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K. NEUTRON SCATTERING

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

Liquids. — Neutron and X-ray diffraction results obtained for *liquid carbon dioxide, CO_2*, have been modelled by means of the reverse Monte Carlo method. Partial pair correlation functions, centre–centre pair correlation functions and relative orientations of molecular axes as a function of distances between molecular centres have been calculated from the models. It was found that well defined orientational correlations exist in the liquid state. Close to the critical point, these correlations seem to disappear, but further away from the critical point, in the high density supercritical state, they reappear. Using large particle configurations, the density fluctuations close to the critical point could be visualized, as demonstrated by Figure 1.

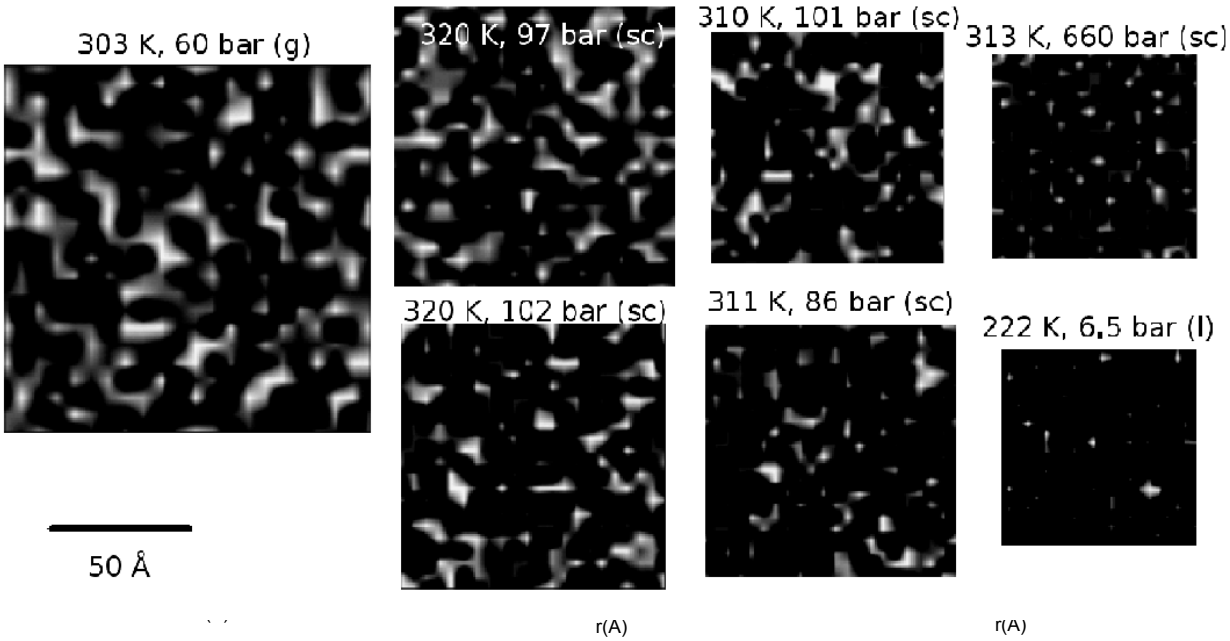

Fig. 1. *Two-dimensional projections of atomic density maps for gaseous (g), near-critical and high density supercritical fluid (sc) and normal liquid (l) CO_2. The pictures were taken on 3–4 Å thick layers (depending on the edge length of the simulation cell), containing roughly 240 molecules.*

The coherent static structure factor of *water* has been investigated by polarized neutron diffraction. Polarization analysis allows us to separate the huge incoherent scattering background from hydrogen and to obtain high quality data of the coherent scattering from four different mixtures of liquid H_2O and D_2O. Consistency with existing partial radial distribution functions, derived without the application of polarized neutrons, was checked by incorporating them into our reverse Monte Carlo calculations. It appeared that the partials from the literature are not entirely consistent with our new polarised neutron data.

Reverse Monte Carlo calculations have been carried out to model the structure of *aqueous RbCl solutions*, as a function of salt concentration. Neutron and X-ray diffraction data were combined with various constraints concerning the coordination of chloride anions. It could be established that increasing ionic concentration causes increasing distortions to the hydrogen bonded network of water molecules—that is, RbCl is a ‘structure breaker’, although to a smaller extent than, for instance, LiCl. For the Rb cations a quite well

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defined coordination sphere was found, particularly at higher concentrations. The orientation of water molecules around the cations may be characterized by a broad distribution of Rb . . .O–H angles, peaking around the tetrahedral angle. This indicates that cations have a weak tendency to occupy a position close to one of the lone electron pairs of the O atoms. It was also found that in the rather vaguely defined hydration shell of chloride ions, six (or somewhat more) water molecules may surround each anion. However, on average, only about three of them point straight towards the anion with one of their H atoms, whereas all other hydrogens are turned away from the ion. The six neighbouring water molecules of the hydration shell can thus be separated into about three hydrogen-bonding and three (or four) non-H-bonding water molecules.

Chalcogenide glasses. — The structure of sputtered amorphous $Ge_2Sb_2Te_5$ was studied by Te-, Sb- and Ge K-edge EXAFS, X-ray diffraction and, for the first time, neutron diffraction. The five datasets were modelled simultaneously by the reverse Monte Carlo simulation technique. The results obtained are thus consistent with all of the five measurements. Within the experimental errors the coordination number of Te, Sb and Ge is 2, 3 and 4, respectively. Thus, in contrast with the findings of some recent works on amorphous $Ge_2Sb_2Te_5$ all atoms satisfy the 8-N rule. Besides Te-Ge and Te-Sb bonds present in the crystalline phases Ge-Ge and Sb-Ge bonding was also found to be significant.

The atomic structure of the binary AsSe, ternary $(AsSe)_{80}Ag_{20}$, $(AsSe)_{85}I_{15}$ and quaternary $(AsSe)_{65}(AgI)_{35}$ glasses has been studied with the X-ray and neutron diffraction. The local order was also probed with EXAFS at the Ag, As, I and Se K-edges. All experimental data were modelled simultaneously by the reverse Monte Carlo technique. Ag and I modify the structure of the host matrix (AsSe) in opposite ways. Ag atoms are preferentially covalently bonded to Se. Addition of I to AsSe decreases the connectivity of the matrix. The average coordination number in amorphous $(AsSe)_{85}I_{15}$ $<N> = 2.18 \pm 0.2$. I atoms are covalently bonded to As atoms.

Metallic glasses. — Short range order of amorphous $Mg_{60}Cu_{30}Y_{10}$ was investigated by X-ray and neutron diffraction, Cu and Y *K*-edge X-ray absorption fine structure measurements and by the reverse Monte Carlo simulation technique. We found that Mg-Mg and Mg-Cu nearest neighbour distances are very similar to values found in crystalline Mg_2Cu. The Cu-Y coordination number is 1.1±0.2 and the Cu-Y distance is ~4% shorter than the sum of atomic radii suggesting that attraction between Cu and Y plays an important role in stabilizing the glassy state. Thermal stability and structure evolution upon annealing were also studied by differential scanning calorimetry and in-situ X-ray powder diffraction. The alloy shows a glass transition and three crystallization events, the first and dominant one at 456 K corresponding to eutectic crystallization of at least three phases: Mg_2Cu and most likely cubic MgY and CuMgY.

Borosilicate glasses. — The network structure of multi-component borosilicate based waste glasses with composition $(65\text{-}x)SiO_2 \cdot xB_2O_3 \cdot 25Na_2O \cdot 5BaO \cdot 5ZrO_2$, x=5-15mol% (host glass) was studied by high-Q neutron diffraction. For data analyses both the direct sine-Fourier transformation and reverse Monte Carlo simulation was applied. Several atomic partial correlation functions are displayed in Figure 2. It was established that the Si-O network consists from tetrahedral SiO_4 units with characteristic first neighbour distances $r_{Si\text{-}O}$=1.60 Å and $r_{Si\text{-}Si}$=3.0 Å. The boron surrounding contains two well-resolved B-O distances at 1.40 and 1.60 Å and, both 3- and 4-fold coordination are present. A chemically mixed network structure is proposed including $^{[4]}$B-O-$^{[4]}$Si and $^{[3]}$B-O-$^{[4]}$Si chain segments. The O-O and Na-O distributions suggest partial segregation of silicon and boron rich regions. The

highly effective ability of Zr to stabilize the glass and hydrolytic properties of sodium-borosilicate host materials is argumented by the network forming role of Zr ions. Uranium-loaded glasses have been successfully prepared, and it was found that they posses good glass and hydrolytic stability. Our neutron diffraction data are consistent with a model where the uranium ions are incorporated into interstitial voids in the essentially unmodified network structure of the starting host glass. The U-O atomic pair correlation functions show a sharp peak at around 1.7 Å, and several farther smaller intensity but distinct peaks are between 2.8- 4.1 Å. Uranium ions are coordinated by 6 oxygen atoms in the 1.6-3.4 Å interval.

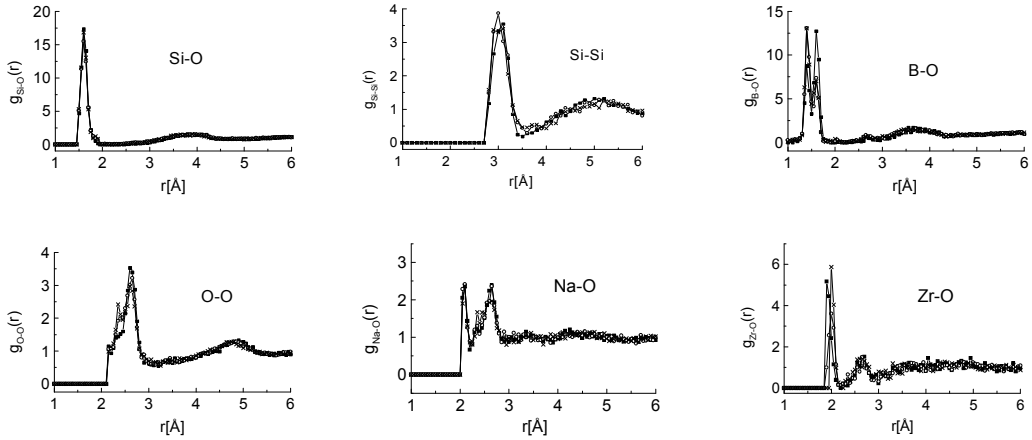

***Fig. 2**. Comparison of several partial correlation functions obtained by RMC modelling for the multi-component borosilicate glasses: B5 (square), B10 (open circle), B15(crosses).*

Internal stress - In the frame of non-destructive testing project of supercritical water (374 ºC, 221 bar) we have tested the structural parameters of the special containers prepared from iron. The Fe(110), Fe(200), Fe(220) Bragg-reflections were measured from room temperatures up to 400 ºC on several parts of the containers. From the shift of the peak positions - taking into consideration the thermal shift - we have determined the stresses caused by the supercritical water. Figure 3 illustrates the Fe(110) pattern taken at ambient temperature and at 400 ºC; from the data analysis 95 MPa internal stress was calculated, which is significantly lower than the expected Yield strength of 250 MPa.

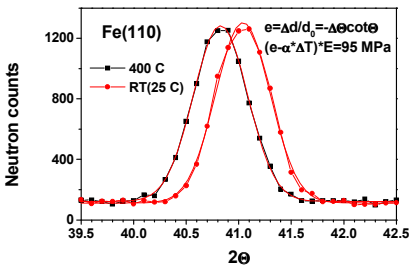

***Fig. 3**. Neutron diffraction pattern of iron container used for supercritical water study*

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Grants and international cooperations

OTKA T 042495 Neutron diffraction study of atomic and magnetic structures (E. Sváb, 2003-2007)

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)

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

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L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, P. Dombi, S. Varró, N. Kroó

Theoretical research. — We have analysed the reflection and transmission of a few-cycle femtosecond Ti:Sa laser pulse impinging on a metal nano-layer. It has been shown that in general a non-oscillatory frozen-in wake-field appears following the main pulse with an exponential decay and with a definite sign of the electric field. The scattering of a laser pulse impinging on a thin plasma layer has also been analysed at relativistic intensities. The nonlinearities originating from the relativistic kinematics of the electrons lead to the appearance of higher-order harmonics in the scattered spectra. In this system we have found significant carrier-envelope phase difference effects. In the frame of our investigations concerning the physics of surface plasmon polaritons, we have worked out a new model which confirms the existence of enhanced electromagnetic fields bound to a thin metal layer evaporated on a glass substrate. Our latest result in attophysics has been to show 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 “collaps bands”, where the electron current is erratic or noise-like, and there exist “revival layers”, where the electron current consist of ultrashort pulses of attosecond duration. The attosecond structure of the electron photocurrent can, perhaps be used for monitoring ultrafast relaxation processes in single atoms or in condensed matter.

We have worked out the theory of high-density black-body radiation on the basis of the new concept of binary photons which satisfy the exlusion principle, thus they behave like fermions. We have derived explicit expressions for the Wigner function of wave functions in arbitrary high D dimensions which depend on the hyperradius – that is, of s waves. Due to the constraint on the dependence of the s wave on the coordinates, s waves describe entangled quantum systems. Since an isotropic Bose-Einstein condensate is described by an s wave, the Wigner function provides a deeper insight into the physics of these states and, in particular, correlations between position and momentum spanning quantum phase space. In the context of quantum optics, we have analysed 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 has been assumed that there is always only one photon present in the measuring apparatus during one elementary experiment. It is explicitely shown in several examples that the bunching and anti-bunching of the counts in serieses of elementary single-photon experiments is governed by the statistical properties of grouping the sequences of the elementary measurements.

Experimental research. — Surface plasmons (SPO) have been in the centre of our interest for many years. Our recent experiments concentrated on their behavior in extremely high laser fields, produced by short pulsed (2ps, 120 fs) titanium-sapphire lasers. The laser pulses excited the SPO-s in resonance conditions and the light emitted by them was analyzed, both its angular distribution and spectrum. Second harmonic (at 395nm) and around it a broad fluorescent spectrum was found, as seen in Fig. 1. The former one is p-polarized as the exiting light, while the latter one is depolarized. The real

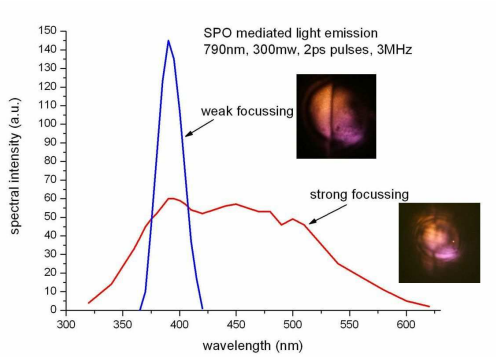

Fig. 1 *Characteristics of surface plasmons on Au*

origin of this broad spectrum, similarly as the distorted light spot in reflection, occurring at the same laser power density where this light occurs is not yet completely understood.

We also published several experimental results related to our 2006 research in femtosecond laser pulse generation and compression. We have upgraded the pump laser of the existing novel laser oscillator delivering 200 nJ pulses to a commercial solid-state system. A pair of novel transmission gratings was inserted as the pulse compression stage for this oscillator.

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Grants and international cooperations

OTKA T048324 Theoretical and experimental study of the newest nonlinear processes of 'attophysics' generated by superintense laser fields within the light wavelength and oscillation period scales (S. Varró, Gy. Farkas 2005-2007)

OTKA IN 64303 Investigation of laser-induced ultrafast processes on metal surfaces, Bilateral cooperation with the Max-Planck-Institute for Quantum Optics, Garching, Germany (S. Varró, P. Dombi, Gy. Farkas 2006-2007)

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

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 chirped-pulse Ti:sapphire 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

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L.2. Varró S; Irreducible decomposition of Gaussian distributions and the spectrum of black-body radiation; *Physica Scripta*; **75**, 160-169, 2007

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L.10. Dahl* JP, Varró S, Wolf* A, Schleich* WP; Weyl-Wigner correspondence in two space dimensions; *Journal of Modern Optics*; accepted for publication

L.11. Kroó N, Varró S, Farkas Gy, Oszetzky D, Nagy A and Czitrovszky A; Quantum metal optics; *Journal of Modern Optics*; accepted for publication

L.12. Varró S; Correlations in single-photon experiments; *Fortschritte der Physik*; accepted for publication

L.13. Varró S, Farkas Gy; Attosecond electron pulses from interference of above-threshold de Broglie waves; *Laser and Particle Beams*; accepted for publication

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L.14. Kroó N; Fényes új világ: egy új típusú fény és alkalmazásai (Bright new world: a new type of light and its applications, in Hungarian); *Fizikai Szemle*; **57**, 37-42, 2007

See also P.3.

M. LASER PHYSICS

K. Rózsa, G. Bánó, L. Csillag, A. Derzsi[#], Z. Donkó, P. Hartmann, P. Horváth[#], Z.Gy. Horváth, K. Kutasi, P. Mezei

Computational plasma studies. — We have investigated the electron kinetics in a hollow cathode discharge by a coupled fluid - Monte Carlo model, and through the solution of the Boltzmann equation. Simulations were carried out to uncover the role and effects caused by fast neutral species in low-pressure gas discharges. Such species originate from elastic collisions between fast ions and thermal buffer gas atoms and were found to cause significant excitation of the gas near the cathode and to induce enhanced emission of electrons from the cathode surface. Langmuir probe measurements were carried out in conjunction with numerical simulations to determine basic characteristics of helium glow discharges. The probe measurements have confirmed the presence of a nearly thermal electron population in the negative glow region of the discharge. In the field of strongly coupled plasma physics we have performed molecular dynamics (MD) simulations and investigated thermodynamic and collective properties of (i) classical bipolar bilayer systems, (ii) two-dimensional many-particle system characterized by Yukawa type interaction potential, including studies of the solid-liquid phase transition, as well as the shear viscosity and shear thinning effect in this latter system in the liquid phase.

Hollow cathode lasers. — Near 200 nm deep ultraviolet hollow-cathode metal ion lasers can be used as light sources for UV Raman and laser-induced fluorescence spectroscopy. These lasers are usually excited by charge transfer reactions between noble gas ions and metal atoms. High density of noble gas ions is created in hollow-cathode discharges while the necessary metal atom density can be produced either by thermal evaporation or utilizing the cathode sputtering effect of the discharge. Our recent investigation is focused on the development of a sputtered 224 nm segmented hollow-cathode silver ion laser. A novel discharge arrangement has been developed in order to prolong the lifetime of the laser tube. 220 mW peak power has been achieved using our previous model. Recently we are working towards a practical sealed-off laser version that will be tested for Raman spectroscopic measurements in bio-medical applications.

Electrolyte cathode atmospheric pressure glow discharge (ELCAD). — In a normal and an abnormal ELCAD plasmas the density of electrons (n_e) and positive ions (n^+) were estimated from the earlier measured values of the cathodic current density (j_c), the cathode fall (U_{cf}), the electric field (E_c), the length of cathode dark space (CDS) (d), the kinetic energy (E_{ion}), the last free path of positive ions hitting the cathode (l) and the rate of secondary electron emission (γ). In a normal ELCAD, the density of positive ions forming the space charge: $n^+_{sp} \approx 5.7\times10^{12}$ cm^{-3}, the density of positive ions hitting the cathode: $n^+ \approx 1.1\times10^{12}$ cm^{-3}, the electron density at the cathode: $n_{e,c} \approx 3.7\times10^{11}$ cm^{-3}, the multiplication of electron in cathode dark space $M \approx 15.3$ were obtained, thus the electron density at the end of cathode dark space: $n_e \approx 5.7\times10^{12}$ cm^{-3}. This electron density agrees well with $n_e \approx 7\text{x}10^{12}$ cm^{-3} and $n_e \approx 10^{12}$ cm^{-3} which were obtained in the center of an ELCAD plasma by other experiments.

For abnormal (capillary cell) ELCAD due to its higher j_c, E_{ion}, U_{cf}, l, and shorter d values compared with those of a normal one , $n^+ \approx 4.3\text{x}10^{12}$ cm^{-3}, $n^+_{sp} \approx 2.1\text{x}10^{13}$ cm^{-3} , $M \approx 1.64$, and $n_e \approx 2.1\text{x}10^{13}$ cm^{-3} were estimated. These data indicate that the higher charge density

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values in an abnormal ELCAD are mainly produced through the enhanced rate of secondary electron emission and not through an increased ionization in a shorter CDS. These values are lower by 1-1.5 order of magnitude than that obtained from the measured Stark-broadening of the emitted H_β=486.1 nm line. The possible reason of this significant difference may be that, the Stark broadening method using H_β=486.1 nm emission line can be used with acceptable reliability for determination of n_e only if n_e is larger than 10^{15}–10^{16} cm^{-3}.

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 Sciences, supported by a GVOP grant. The „pre-industrial" application of the prototype starts in Germany at the end of this year.

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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-OTKA-NSF 90/46140 Strongly coupled Coulomb systems (Z. Donkó, 2005-2007)

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 T-042493 The role of the ions of the basic electrolyte solution in the electrolyte cathode atmospheric glow discharge (P.Mezei, 2003-2007)

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

GVOP-3.1.1.-2004-05-0435/3.0 Multispectral imaging reflectometer (M.Fried and Z.Gy. Horváth, 2005-2007)

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M.9. Mezei P, Cserfalvi* T; Charge densities in the electrolyte cathode atmospheric glow discharges (ELCAD); *Eur Phys J Appl Phys*; **40**, 89-94, 2007; DOI: 10.1051/epjap: 2007123

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M.11. Hartmann P, Donkó Z, Kalman* G J; Numerical experiments on complex plasmas: 2D Yukawa systems [invited lecture]; In: *Proc. of 28th International Conference on Phenomena in Ionized Gases, July 15-20, 2007*, Eds.: Schmidt J, Simek M, Pekarek S, Prukner V; Prague, Czech Republic; T04, 2007

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Patents

M.14. Medical application of lasers (Z. Gy. Horváth; E-D Medical Laser Center)

O. LASER APPLICATION

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

Optical measuring techniques. — This year we finished two National Research and Development Projects on Environmental Pollution of the Atmosphere and on Nanotechnology.

In the frame of the **NRDP 089/2004** (National Research and Development Program) - **Atmospheric Pollution of the Atmosphere-,** we finished the development of two airborne particle counters and sizers and we calibrated a dual wavelength optical particle spectrometer (DWOPS) enabling simultaneous measurement of the concentration, size distribution, refractive index and absorption of the aerosol particles. These parameters can help us in determination of the origin of the measured aerosol contamination and give more complete information about the particles to be measured than any existing device in this field. The other benefit of the developed devices 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. Using the airborne particle counters 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.

The new DWOPS system with increased sensitivity and resolution was calibrated within the frame of a common Hungarian-Austro-German-American workshop organised in our institute. The calibration was made not only for the size and concentration, but also for the real and imaginary part of the refractive index of the aerosol particles. A new software package was developed for the control of the measurement the 3D display of the measured data and their evaluation.

During the measurement campaigns performed using the mobile laboratory air contamination maps were composed in several districts within the city of Budapest and its surrounding. Databases containing all collected results were analyzed. 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 the case of diseased airways.

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

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

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In the frame of the **NRDP 071/2004 – Nanotechnology Program** we developed a high resolution phase shifted surface testing interferometer which can measure not only stationary surfaces but also thermal and elastic deformations with sub-nanometer resolution.

The tested surface can be recovered by fast evaluation of four interferograms shiftet by $\pi/4$ using a special software developed for 3D surface mapping. This system is also suitable for investigation of submicron aerosol particle sediments on different surfaces.

In the frame of **GVOP - 3.1.1-2004-05-040/3.0** project a submicron resolution X-Y camera positioning system was developed and optimized for registration of digital holograms. Registration of the hologram in 64 sub-holograms in stepping/scanning mode and stitching of the obtained images makes possible to increase the virtual resolution of the obtained hologram and the size of the sample to be tested. A patent for this new technique was elaborated and applied.

In the frame of **GVOP- 3.1.1-2004-05-0259/3.0** project the dynamics of the photochemical catalytic decomposition of toxic ingredients was investigated using light scattering method. An UV excitation system for enhancement of the chemical decomposition was designed.

Measurement of the statistics of photons generated in nonlinear optical processes were performed in the case of surface plasmons, parametric deconversion etc. The statistics of the excitation light and the light generated by surface plasmons was compared.

Experimental and theoretical studies of the statistical properties of surface plasmon polaritons (SPO-s) were studied. Both classical and non-classical properties of surface plasmons were analysed. The temporal statistical behaviour at low excitation level, measured by detecting the SPO emitted photon statistics as expressed by the correlation function and the temporal photon count distribution, shows that the SPO-s preserve the photon statistics of the laser. Independent simple model calculations confirmed the existence of enhanced E.M. fields of surface plasmons.

Amorphous carbon thin layers. — Our research work was focused on the investigation of structure and properties of different carbon-based materials and their possible applications. The tuning of the emission photon energy of amorphous carbon films prepared from benzene plasma was achieved by changing the deposition self-bias. The photoluminescence maxima were correlated to definite structural units of the films. We have developed lithium intercalated electrodes for rechargeable batteries based on carbon black and amorphous carbon mixture. Nano-diamond thin films represent a new direction in the research field of carbon-based materials. We have started to study the dependence of bonding and electronic properties of these materials on the grain size.

Nowadays nanocrystalline (NCD) and ultra-nanocrystalline diamond (UNCD) thin films are promising materials of modern technology due to their unique and advantageous mechanical, electrochemical, electronic and optical properties. These layers have composite structure where the diamond crystallites are embedded into an amorphous carbon matrix. Beside the average grain size the properties of the grain boundaries are the most important factors affecting the film properties. Generally the grain boundaries are the interface region between the two (crystalline diamond and amorphous carbon) phases, but in the case of UNCD films of small grains the inter-grain amorphous phase is so thin that the entire of it constitutes the grain boundary.

Our aim was to investigate the structure of the grain boundaries of these materials in detail, focusing on the uniformity and on the grain size dependence of the structure.

Raman spectroscopy is widely used for the characterization of these materials. However it is rather difficult to obtain specific information on the bonding configuration of only the grain boundaries from Raman spectra of NCD thin films. These spectra give averaged information about the bonding configuration of all carbon atoms falling into the excitation volume being a part of the diamond crystallites or the surrounding amorphous matrix. Additionally the resonance enhancement of the scattering in the amorphous matrix causes the intense bands of this phase to overlap the scattering contribution of such minor parts of the structure, like the grain boundaries.

To overcome these difficulties and to obtain information on the bonding configuration in grain boundaries from the Raman spectrum of NCD films we have lowered the excitation volume so that the excitation took place only on a few crystallites. Additionally the excitation energy was shifted in order to decrease the resonant Raman scattering. This way the characteristic vibrations from grain boundaries of NCD thin films of different grain size were detected successfully (Fig. 1) and identified as characteristic bands of aromatic hydrocarbons and sp^3 CH_2 groups.

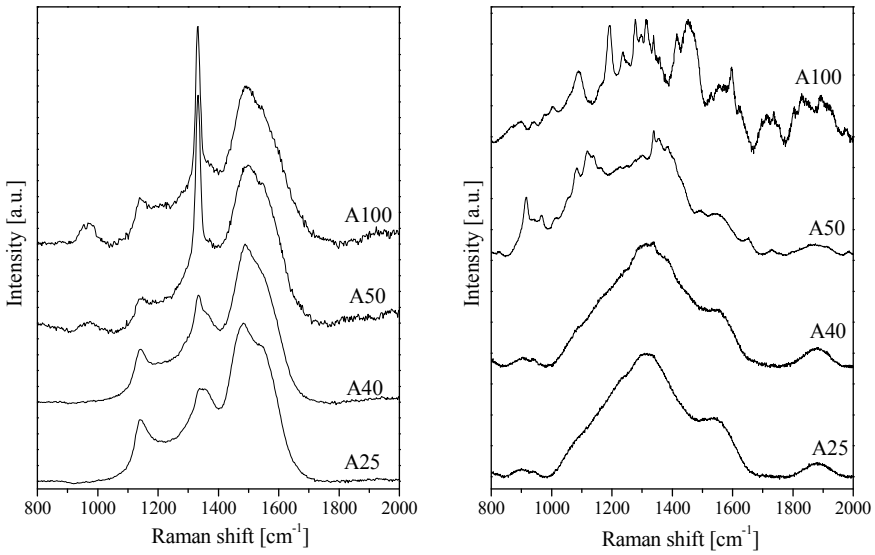

Fig. 1. *488 nm (a) and 785 nm (b) excited Raman spectra of ultra-nanocrystalline diamond films of different grain size: A25, A40, A50 and A100 samples have grain sizes between 3-50 nm, 50-100 nm, 100-150 and 200-300 nm respectively.*

The above described method cannot be used for UNCD films having grain sizes below 50 nm, since excitation beam diameter is limited by the diffraction. In the case of these layers we have used Surface Enhanced Raman Scattering (SERS) to detect characteristic vibrations from grain boundaries. Putting SERS-active gold nanoparticles (average size is 20 nm) in contact with the UNCD film, the excitation volume from where the SERS signal arises is limited to a few tens nm surrounding of these nanoparticles. As a result, we were able to detect characteristic vibrations of the grain boundaries of UNCD thin films too.

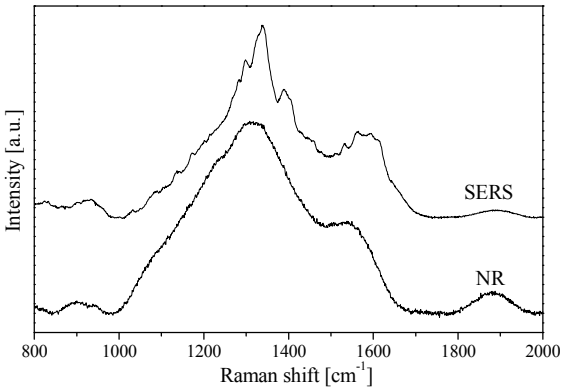

Fig.2. *Comparison of the normal (NR) and surface enhanced (SERS) spectra measured on the A25 sample.*

The detailed analysis of the spectra measured on the same UNCD sample showed also that the position and the intensity of some of the observed peaks varies when measuring in different points of the surface. Statistical analysis was performed on more than 100 spectra recorded in different points of the sample. The most frequent peaks and corresponding structural units were determined. Our results show that the Raman scattering with near-infrared excitation is highly sensitive to smallest differences in the structure and it allows the detection and determination of the Raman peaks arising from definite regions of the sample.

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Grants and international cooperations

NKFP-3A/089 National Research and Development Program, Environmental Pollution of the Atmosphere (Coordinator: A. Czitrovszky, 2004-2007)

NKFP- 3A/071 National Researh and Development Program, Nanotechnology II (sub-coordinator: A. Czitrovszky, 2004-2007)

OTKA T-043359 Preparation and complex characterization of carbon based nanocomposites (M. Koós, 2005-2007)

GVOP-3.1.1. No 0403/3.0, DIADEM (in cooperation with Budapest Technical University) (A. Czitrovszky, 2005-2007)

GVOP-3.1.1. No 0259/3.0 Photo-catalytic decomposition of pollutants (in cooperation with the University of Szeged (A. Czitrovszky, 2005-2007)

Bilateral Austro-Hungarian Cooperation, Contract No A-20/01 (A. Czitrovszky, 2005-2007)
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O.18. Szymanski* WW, Golczewski* A, Angy* A, Gál P, Czitrovszky A; An innovative approach to optical measurement of atmospheric aerosols – Determination of the size and complex refractive index of single aerosol particles; In: *Advanced Environmental Monitoring*; Eds.: Y.J. Kim, U. Platt, Springer; pp. 167-187, 2007

See also L.10.

P. FEMTOSECOND LASERS

R. Szipőcs, Á. Bányász, J. Fekete, P. Antal

Design of leaking mode free hollow core photonic bandgap optical fibers. — Photonic bandgap (PBG) fibers are optical fibers that have unique optical properties compared to step-index and graded index fibers. Hollow-core (HC) PBG fibers are expected to have lower loss than total-internal-reflection guiding fibers because of the lower absorption and Rayleigh-scattering of air compared to glass. The intensity threshold for nonlinearity can be several orders of magnitude higher for these fibers compared to silica-core fibers, which allows the propagation of high intensity laser pulses without significant spectral distortions. The dispersion of these fibers is also unique and varies strongly across the bandgap. The shape of the dispersion profile of these fibers is similar to that of one-dimensional (1D) photonic bandgap structures or quarter-wave stacks and two-dimensional (2D) PBG structures.

Present HC PBG fibers are not ideal for ultrafast laser applications: they exhibit limited bandwidth compared to the tunability range of Ti:sapphire lasers (670 nm to 1060 nm) and their dispersion varies with wavelength. Some progress on producing ultrabroadband, all-silica PBG fibers, which have almost an octave bandgap, has already been made. The so-called all-silica Bragg fiber may exhibit a very wide bandgap if one only takes into account the alternating fused silica and air layers. However, the realized fiber with the additional silica struts, which set the spacing between the silica rings, increases the effective refractive index of the low index cladding regions above unity.

This small modification of the low index layer introduces plenty of interface-mode anti-crossing events which rive the bandgap to many smaller ones and dramatically reduce the usable bandwidth. Some effort on broadening the usable bandgap has been made by searching for an optimum air-filling fraction of the fiber by changing the core size and the thickness of the first silica layer in a realistic HC PBG fiber or introducing anti-resonant structures around the core. Algorithms that are capable of such simulations – such as finite-element method (FEM), – are very timeconsuming and ineffective in designing HC fibers when the optimum structure is maintained from transmission maps calculated in small steps and covering wide ranges of parameters.

This year we investigated the physical origin of the so called ”leaking modes” in all kind of PBG fibers including HC fibers with cylindrical or hexagonal fused silica cladding structures, or in any kind of PBG structures. We found that when meeting the so called quarter-wave condition requirement in the design at the center of the desired bandgap, the bandgap is free of leaking modes: properly taking into account the contribution from the silica struts (which results in a few percent change in the effective refractive index of the air spacer layers) in all-silica Bragg fibers, we can construct structures exhibiting an ultra-large bandwidth (a few hundreds of nanometers). For 1D simulations, we used the well known transfer matrix method to describe the physical properties of the Bragg fiber. Later on, we applied the FEM for making simulation on the real, 2D structures including the effect of fine structures such as the fused silica struts.

We pointed out that two kinds of loss mechanisms are distinguished for HC PBG fibers. While ”leaking modes” are due to the high standing wave field in the air spacer layers and can be removed by correct design of the structure, some ”surface modes” still appear in the silica struts due to symmetry concerns and cannot be described by 1D models.

In our following numerical examples, designs comprising 3 silica-air layer pairs are presented which support bandgap guidance around 1 μm. 1D simulation results are shown in Fig. 1 (a). The ideal design in which the index rising effect of the support bridges in the air spacer layers is neglected is shown with a dashed line.When the small index rising effect of silica struts is taken into account but the spacer thickness is not corrected, leaking modes appear in the bandgap. This curve is shown with dotted line. The correct quarter-wave design exhibits a broad bandwidth free of leaking modes (shown with solid line).

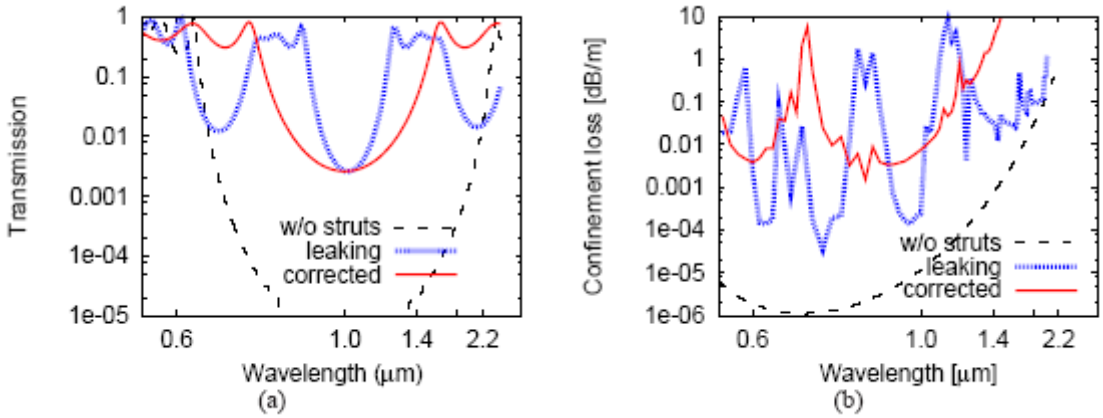

Fig. 1 *(a) 1D computation results for transmission (corresponding to the loss of the fiber) as a function of wavelength for PBG structures of the following designs:* n_L *=1.00 and* $PT_L = \lambda_0/4/\cos(\Theta_0)=3.584$ *μm,* Θ_0 *=86°, exhibiting a very wide bandgap (dashed line),* n_L *= 1.02 and* PT_L *= 3.584 μm with the leaking modes destroying the bandgap (dotted line),* n_L *= 1.02 and* $PT_L = \lambda_0/4/1.02/\cos(\Theta_2) = 1.175$ *μm restoring the bandgap to some degree (solid line), and (b) corresponding FEM results*

Corresponding FEM calculation results performed by our partners at Furukawa Electric Technology Institute (FETI) are shown in Fig. 1 (b). The FEM simulation was carried out on an analogue structure consisting of a 6 μm core, 3 alternating layers of silica and air, and 12 silica struts of 50 nm thickness in each air layer. The properly designed structure is free of ”leaking modes” however some perturbation due to still existing ”surface modes” can be observed.

As a conclusion, we can say that optical performance of HC Bragg fibers is extremely sensitive to the effect of support bridges between the concentric fused silica rings. In spite of the fact that they modify the effective refractive index of the air spacer layers by a few percent only, proper readjustment of physical thicknesses meeting the well known quarter-wave condition may require as high as 70% changes in these parameters.We found that this is typical for grazing incidence ($\theta \approx 84°$ to 87°) in 2D and 1D photonic bandgap structures as well. A 2D finite element method and a 1D equivalent thin film analysis show, however, that leaking modes or mode anti-crossing events can be avoided by proper modeling and choice of the physical layer coefficients, when optical thickness of each layer is set to $\lambda_0/4$.

The presented results and the applied numerical methods can be applied for modeling and design of all kinds of photonic bandgap fibers.

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Grants and international cooperations

OTKA T-049296 Propagation of ultrashort laser pulses in photonic crystal fibers and fiber amplifiers (R. Szipőcs, 2005-2007)

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 contract on „Research and development of femtosecond pulse pump-probe spectroscopic system, (Coordinator: R. Szipőcs, 2006-2007)

Publications

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P.1. Várallyay* Z, Fekete J, Bányász Á, Szipőcs R; Optimizing input and output chirps up to the third order for sub-nanojoule, ultra-short pulse compression in small core area PCF; *Appl Phys B*; **B86**, 567-572, 2007

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See also L.7., L.8.

Q. OPTICAL THIN FILMS

K. Ferencz

Optical thin film structures consisting of nanoscale laminated layers. — We have continued our research concerning the development of optical thin film structures containing nanooptically thin layers for advanced applications in laser physics and information technology. We have refined our new electron-beam deposition technology for the production of optical coatings containing nanooptically thin titania, silica, tantala, alumina, hafnia layers. Using needle-like optimization thin film design method, we have continued our research concerning the development of many kinds of ultrafast nanooptical coating systems – ultra-wide-band, low dispersion antireflection coatings, low dispersion beamsplitter coatings, ultrafast dichroic mirrors, wide-band output coupler mirrors, spectral shape filters for amplifiers, for example. We have found a new application of our nanooptically thin indium-tin-oxide (ITO) layers deposited with reactive e-beam method in integrated optical sensor chip technology. Our thin ITO layers having electrical resistance in the kohm range were successfully applied on the top of waveguide structures, because their optical absorbance is very low in the red part of the visible spectrum. Using our new deposition technology we have developed special type wide band ultrafast front polarizer coatings for the UV, VIS and IR ranges. We have developed new trichroic polarizer beam splitter coating working at 45 degree angle of incidence. This coating has high reflectance for the s-polarized light and high transmittance in three separated bands (blue, green, red) for the p-polarized light in the visible range. The application of our new trichroic polarizer looks very promising in the 3D display technology. Our work on interference filters is still in progress for high sensitivity detection of protein molecules elaborated by gene manipulation methods.

Other developments on optical coatings. — Our work on ultrafast optical coatings is still in progress cooperating with the Max-Planck-Institute for Quantum Optics, Garching, Germany (Prof. Ferenc Krausz) for many types of advanced applications in laser oscillators, amplifiers, autocorrelators, coherent X-ray generation, etc. We have developed small-scale optical manufacturing technology for producing of large size fused silica compensating wedges having a few tenths of millimeter minimal thicknesses. We have arranged a new optical coating laboratory infrastructure financed by company Optilab Ltd. in our campus, where a new optical coating machine type INTEGRITY 36, manufactured by the US company DENTON VACUUM will start its operation in the near future. Our new coating machine manifests the state-of-the-art optical coating technology, the combination of ion-assisted deposition technology, oil-free cryopumping and a sophisticated computer control system.

Based on our standard multiple-beam interference method for analysing optical coatings we have developed a new fast quantitative technique for analysing thin mineral oil films on water surfaces (project „Aquanal”). Using our CCD array spectrometer we have investigated the spreading phenomena of different kind of oil materials on water surfaces, and we have found that the equilibrium thicknesses of the oil films in many cases are much more thicker than the monolayer thicknesses are. We plane to continue our research in this field using new type oil samples to understand the details of the interaction between mineral oils and water surface. Based on our investigations we have developed optical multilayers useful as cheap sensors in oil contamination detection tasks.

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

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Contract

OPTILAB-SZFKI No. 1653/2007

Grants and international cooperations

NKFP3A/0005/2002 Nanobiotechnology: Elaborate a method to build nanotechnological devices for use in biology (Coordinator: P. Ormos, Szeged, participant: K. Ferencz, 2002-2007)

NKFP3A/071/2004 Nanotechnological material modifications and their metrology (Coordinator: J. Gyulai, MTA MFA, participant: K. Ferencz, 2004-2007)

NKFP3A/079/2004 On-site analysis of natural waters, geological media by micro- and nano-sensation methods („Aquanal") (Coordinator: I. Bársony, MTA MFA, participant: K. Ferencz, 2004-2007)

Publications

See J.32.

R. GROWTH AND CHARACTERIZATION OF OPTICAL CRYSTALS

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

Growth and study of nonlinear yttrium-aluminium-borate (YAB) crystals. — Optical hyperfine structures (OHS) were detected in Ho-doped YAB single crystals at 9K by high resolution (0.01 cm^{-1}) Fourier Transform (FT) spectroscopy. This was a rare co-incidence of high optical quality of the crystals, the extreme resolution of the spectrometer, the single site, tension free incorporation of the dopant, the proper symmetry of the crystal field around the Ho^{3+} ions (trigonal prismatic, D_3 Yb-sites), and the 100% natural abundance of the ^{165}Ho isotope (I=7/2 magnetic moment). Only three other optical crystals are known in the literature ($LiYF_4$, CaF_2 and $CsCdBr_3$) where Ho^{3+} related OHS were experimentally demonstrated, and those observations were restricted to the $^5I_8 \rightarrow {}^5I_7$, $^5I_8 \rightarrow {}^5I_6$, and $^5I_8 \rightarrow {}^5F_5$ transitions. In YAB:Ho OHS was identified in transitions from the ground state $^5I_8$ to the $^5I_7$, $^5I_6$, $^5I_5$, $^5F_5$, $^5S_2$, $^5F_4$, $^5F_3$, and $^3K_8$, manifolds. According to the theoretical predictions the number of the split OHS components depended on the degeneracy of the initial and final state of the transitions. Also, the separation of the OHS components was in accordance with the calculated values (0.1-0.2 cm^{-1}). The crystal field calculations were in good agreements with the experimental energy levels of all the manifolds in the investigated 4000-23000 cm^{-1} range, including their Stark components.

Growth and study of lithium- and potassium/lithium- niobate single crystals with different compositions and doping. — The room temperature stability region of the tetragonal tungsten bronze-type potassium lithium niobate ($K_3Li_2Nb_5O_{15}$, KLN) has been determined by X-ray phase analysis on ceramic samples synthesized by solid state reaction in the composition range of [K_2O] = 28-33 mol%, [Li_2O] = 12.5-20.5 mol% and [Nb_2O_5] = 50.5-55.5 mol%. Lattice parameters and temperature dependence of the dielectric constants were measured on single phase samples. The axial a/c ratio of the cell parameters, the density and the Curie temperature of the ferroelectric samples have been found predominantly characteristic for the Nb_2O_5 content, varying progressively between 3.11-3.14, 4.431-4.596 g/cm^3 and 492-460 ^oC, respectively. The results are discussed from the points of view of defect chemistry and phase stability. The concentration of intrinsic defects formed primarily by antisite Nb atoms at Li sites has been estimated on the basis of "alkali cation vacancy formation model".

A simple and accurate (~0.02 mol%) spectroscopic method was developed to determine the $LiNbO_3$ crystal composition close to the stoichiometric region based on the evaluation of the vibrational spectrum of hydroxyl ions which always present in air-grown crystals. It was shown earlier that the intensity ratio of the two infrared band components peaking at about 3480 and 3465 cm^{-1} ($R = I_{3480} / I_{3465}$) changed linearly with Li_2O content in the 49.7 – 50.0 mol% range. It was discovered that R depends also on the age of the crystal. However, a simple thermal treatment at about 1000 ^oC was found suitable to return the crystal to its as-grown state. Thus the spectroscopic test can be applied for $LiNbO_3$ crystals of unknown thermal history.

The role of Mg, Y and Mg+Y co-doping in the formation of periodically poled domain (PPD) structure of the congruent $LiNbO_3$ single crystals has been investigated. Crystal were grown by the off-centered Czochralski method, both with X and 148^o Y pulling directions. The developed domain structures were examined on chemically etched slices

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by optical microscopy. While in Y_2O_3 doped crystals PPD structures with irregular boundaries were detected for all concentrations of the solubility range (<0.6 mol%), the formation of domain pattern of MgO doped crystals depended on the concentration. Doping with near-threshold concentration of MgO (5-5.5 mol%) required for the preparation of photorefractive damage resistant crystals only few needle–like domain, below (< 4 mol%) and above threshold (<6 mol %) irregular, patchy-like domain structures were formed. In double doped crystals similar correlation has been observed between the evolution of the PPD structure and the MgO concentration added. The benefit of Mg+Y co-doping manifested both by improving the regularity of the formation PPD structures and the increase of the laser resistance of the crystals. Results have been explained by the impact of the MgO concentration on the magnitude of the coercive field responsible for the local poling processes.

Growth and study of bismuth tellurite (Bi_2TeO_5) crystals. — Yb- and Tm doped Bi_2TeO_5 single crystals were grown by the diameter controlled Czochralski technique. The low temperature absorption spectra of Bi_2TeO_5:Yb consists of three band groups around 10230, 10480, and 10800cm^{-1}. The complex spectra were attributed to strong electron-phonon coupling and the multisite incorporation of Yb^{3+}-ions to the slightly different Bi-sites. The luminescence of Bi_2TeO_5:Yb was dominated by two narrow lines at 979.5 and 978.2nm, corresponding to the different Yb sites. The experimental lifetime of the excited $^2F_{5/2}$ level was 383μs. The radiative lifetime calculated by the Judd-Ofelt model (678μs) corresponded to 55% quantum efficiency. The emission cross-section was calculated by the Füchtbauer-Landenburg model. Its maximum value was in the Y-polarization ($6x10^{-20}$cm^{-1}), and it was promising for potential laser application.

The room temperature absorption spectra of Bi_2TeO_5:Tm crystals consisted of 4 line groups that were assigned as transitions from the $^3H_6$ ground state to the $^3F_4$ (~5900cm^{-1}), $^3H_5$ (~8300cm^{-1}), $^3H_4$ (~12700cm^{-1}), and $^3F_3$+$^3F_2$ (~14500cm^{-1}) levels. The $^3H_6 \rightarrow {}^1G_4$ transition appeared as a shoulder on the intrinsic absorption edge of the host material (~21300cm^{-1}), but some of the $^1G_4$ crystal field components could be determined from the luminescence excitation spectra. Emission spectra were collected after 476.5nm laser excitation. The strongest emission in the visible region situated in the 15000-15500cm^{-1} range and belonged to the $^1G_4 \rightarrow {}^3F_4$ transition. Another strong emission at 12500cm^{-1} was attributed to the $^3H_4 \rightarrow {}^3H_6$ transition. The room temperature lifetime of the $^1G_4$ and $^3H_4$ levels was 160μs and 14μs, respectively. Their ratio may be proper for laser action. The 0.1%Tm content of the crystal was too small to investigate experimentally the $^3F_4 \rightarrow {}^3H_6$ laser transition, but 1.5ms lifetime could be predicted from the peak intensities of polarized absorption spectra.

Application of analytical methods for optical crystals and other media. — Flame AAS methods were elaborated to determine the composition of undoped and doped (Er/Yb) $GdCa_4O(BO_3)_3$ optical crystals. The samples were powdered and dissolved in HCl, and then measured against matrix-matched calibration standards. For Yb:$GdCa_4O(BO_3)_3$, the crystal/melt segregation coefficient of Yb was found close to unity.

An ion chromatography (IC) method was optimized for separation of acetate, formiate and fluoride ions. Risky concentrations of acetate (122μg/m^3) and formiate (9μg/m^3) have been determined in the air of the Cathedral of Cologne. The concentration, of CO_2, CO, formaldehyde and water vapor were monitored in various sections of a mountain church in the Italian Alps during heating. It was shown, that a novel design consisting of low-temperature heating elements eliminated the adverse effects of the conventional hot air heating system in respect of supply, transport, deposition and transformation of harmful

gases, which affect the preservation of displayed art works. In historic churches in Poland another heating method, the use of electric overhead radiant heaters, was shown to provide localized heat to the given area without adversely affecting the art works. Irradiation of the area at the floor level increased temperature and reduced relative humidity in the church, but hardly affected the surfaces sheltered from irradiation, or being outside the heated area.

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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-DFG bilateral project. Multiplexed volume holographic data storage in bismuth tellurite crystals (Bi_2TeO_5) using nanosecond laser pulses (I. Földvári, 2005 – 2007). Partner: Westfälische Wilhelms-Universität, Münster

HAS-Polish Academy bilateral cooperation program. Growth and spectroscopic investigation of rare-earth-doped nonlinear optical crystals (I. Földvári**,** 2005-2007). 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

Hungarian - Italian Intergovernmental S & T Cooperation Programme. Growth and FTIR spectroscopy of optical crystals (L. Kovács, conributor I. Földvári, 2004-2007). Partner: Universita di Parma.

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HAS-Russian Academy Project 25. Investigation of crystal defects in broad forbidden band crystals (J. Janszky, contributor K. Polgár, 2005-2007). Partner: Joffe Phys. Techn. Institute, RAS, St.Petersburg.

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

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R.18. Samek* L, De Maeyer-Worobiec* A, Spolnik* Z, Bencs L, Kontozova* V, Bratasz* Ł, Kozłowski* R, Van Grieken* R; Impact of electric overhead radiant heating on the indoor environment of historic churches, *J Cultur Herit*; accepted for publication

R.19. 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;* accepted for publication

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See also: S.2., S.3., S.5., S.6., S.10., S.13., S.14., S.15.

S. CHARACTERIZATION AND POINT DEFECT STUDIES OF OPTICAL CRYSTALS

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

Electron beam microanalysis on yttrium aluminum borate (YAB) crystals. — The impurity elements playing a dominant role in the formation of as-grown imperfections of YAB crystals growing from potassium trimolybdate melt-solutions undoped or doped with trivalent ions, were identified by energy dispersive X-ray spectrometry in a scanning electron microscope. These impurity elements were: Mo, K, Si, Ti and Ca.

Computer modelling of defects in $LiNbO_3$. — Using a recently derived interatomic potential, intrinsic and extrinsic defect formation energies have been calculated for $LiNbO_3$ and used to calculate the energies of defect reactions giving rise to the experimentally observed lithium deficiency in the material. Of these reactions, the formation of antisite niobium ions compensated by lithium vacancies was found to have the lowest energy, and this is therefore the predicted intrinsic defect model. Doping of a wide range of divalent and trivalent cations into the material was also considered, and predictions were made of the lowest energy sites for occupation, and the corresponding charge compensation schemes.

Microscopic and Raman spectroscopic investigation of the domain structures in $LiNbO_3$:Y:Mg crystals. — Formation of periodic domain structures in Mg and Y doped and Mg+Y co-doped congruent $LiNbO_3$ single crystals grown by an off-centred Czochralski method in the X and 148° Y pulling directions has been investigated by Raman spectroscopic measurements. A band attributed to the $E(TO_9)$ vibrational mode occurred at about 610 cm^{-1} in the Raman spectra recorded in Z(YY)Z backscattering geometry after chemical etching of a PPLN crystal grown in the X pulling direction. The shift of the $E(TO_8)$ band position at the domain boundaries can be explained by the growth of the intensity of the $E(TO_9)$ band. It was demonstrated by time dependent etching measurements that the increase of the $E(TO_9)$ band is a consequence of periodic step-like forms on the surface of the crystal.

Holography in $LiNbO_3$ crystals and silver halide emulsions. — We developed and optimised a thermal treatment system and method for dehydrating and homogenising the oxidation state of lithium niobate crystals with different compositions. The hydrogen concentration was reduced by about two orders of magnitude in iron or manganese doped congruent and nearly stoichiometric samples, as compared to the as-grown state. Using this method we successfully prepared dehydrated $^6LiNbO_3$:Fe samples (at about 95% of ^6Li) for the investigation of thermal neutron dosimeter applications. Such dehydrated samples were also used to test the holographic scattering method for the determination of the hydrogen concentration.

We adapted the FRIINT program, developed at the Department of Physics of the Budapest University of Technology and Economics (BME), for the evaluation of the interferograms obtained by interference microscopic studies of holographic gratings in Fe-doped $LiNbO_3$ crystals.

The processing of silver halide holographic emulsions, fabricated by the Slavich Company (Russia), has been optimised for recording holograms of the $LiNbO_3$ crystals. These

[#] Ph.D. student

emulsions can be used in a real-time holographic interferometric set-up for the in-situ microscopic observation of the build-up of holographic gratings in $LiNbO_3$.

Hydroxyl ions in potassium lithium niobate crystals. — The OH^- stretch mode spectra have been measured in both ferroelectric (KLN-1) and non-ferroelectric (KLN-2) potassium lithium niobate crystals grown from different melt compositions. O-H bond directions making angles of about 15, 60, and 15 degrees with the c-axis have been determined for the three main OH^- bands in KLN-1 peaking at about 3440, 3500, and 3520 cm^{-1}, respectively. Correlations have been found along the growth axis of the crystal between the decrease of the excess Nb content, the change of the hydroxyl band components at 3440 and 3520 cm^{-1}, and the Raman modes at 540 cm^{-1} and 640 cm^{-1}.

Impurity-centred oxygen tetrahedra in sillenites. — Fundamental and multi-mode transitions of the tetrahedral unit modes (A_1 and F_2) in $Bi_{12}SiO_{20}$, $Bi_{12}GeO_{20}$, and $Bi_{12}TiO_{20}$ sillenite crystals have been studied by measuring Raman scattering and FTIR absorption spectra. The ν_1 and ν_3 frequencies related to the A_1 symmetric and F_2 asymmetric stretching modes, respectively, were obtained for MO_4 and ImO_4 tetrahedral complexes, where M is the host matrix metal, i.e. Si^{4+}, Ge^{4+}, and Ti^{4+} and Im is an impurity substituting for M. The Im considered belong to three different isoelectronic series as a) Al^{3+}, Si^{4+}, P^{5+}, S^{6+}, b) Ga^{3+}, Ge^{4+}, As^{5+}, Se^{6+}, and c) Ti^{4+}, V^{5+}, Cr^{6+}. Ions with different valence charges, as Cr^{4+}, Cr^{5+}, Cr^{6+} and Mn^{4+}, Mn^{5+}, were also considered. Systematic trends were put in evidence for the ν_1 and ν_3 frequency pairs as a function of M (or Im) atomic mass and charge (Fig. 1).

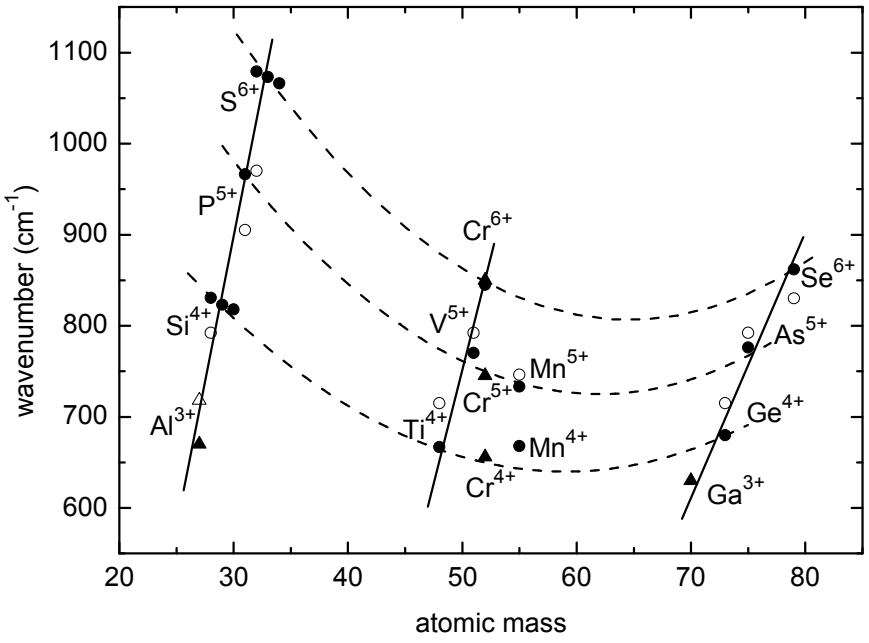

***Fig. 1**. Plot of ν_1 and ν_3 frequencies vs. atomic mass of impurities (Im) for different ImO_4 tetrahedral groups in sillenites. Open symbols: ν_1 (A_1 mode); full symbols: ν_3 (F_2 mode). Circles: our work; triangles: literature.*

Spectroscopy of Cu centres in lithium tetraborate single crystals. — Cu^{2+} centres in the tissue-equivalent thermoluminescent dosimeter material, $Li_2B_4O_7$:Cu, have been shown by electron spin resonance experiments to substitute at the Li^+ site, with an appreciable relaxation of the site and its surroundings. The singly charged Cu^+ centre, showing anomalous optical emission behaviour below 6K, has been shown to occupy off-centre positions displaced from interstitial sites on the twofold symmetry axis connecting B_4O_7

groups of the $Li_2B_4O_7$ lattice. The results are helpful for understanding the radiation induced charge transfer processes.

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, implanting 1.5 MeV N^+ ions with doses in the $10^{16} – 10^{17}$ ions/cm^2 range. The waveguides were studied using the following methods: M-line test, to check the functionality of the samples, interference contrast microscopy, to determine the total modulation of the refractive index in the structures, cathode luminescence (CL), electron diffraction pattern (EDX) analysis, and spectroscopic ellipsometry, to determine the in-depth refracive index profile of the waveguides. The results showed that the waveguides were of barrier-type, i.e. the ion implantation produced a negative refractive index change around the maximum of the distribution of the implanted ions.

History of science. — The collaboration of the Crystal Physics Department and the Crystal Physics Ggroup at the Budapest Technical University was analyzed.

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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)

TéT Italian-Hungarian Intergovernmental S & T Cooperation (I-46/03): Growth and FTIR spectroscopy of optical crystals (L. Kovács, 2004-2007)

TéT Italian-Hungarian Intergovernmental S & T Cooperation (I-15/03): Fabrication of active and passive integrated optical elements and devices by ion beam implantation (I. Bányász, 2004-2007)

HAS – Polish Academy of Sciences joint project: Structure of real crystals (A. Watterich, 2005-2007)

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, contributor K. Lengyel, 2005-2007)

Long term visitor

— Dr Margherita Mazzera, Department of Physics, University of Parma, Italy, 1-31 October 2007 (L. Kovács)

Publications

Articles

S.1. Araujo* RM, Amaral* JB, Jackson* RA, Valerio* MG, Lengyel K, Kovács L; Computer modelling of substitutional defects and optical properties of the ferroelectric and paraelectric phases of $LiNbO_3$; *phys stat sol (c)*; **4**, 1201-1204, 2007

S.2. Hajdara I, Lengyel K, Dravecz G, Kovács L, Péter Á, Polgár K; Spectroscopic methods for the determination of the composition of potassium lithium niobate crystals; *phys stat sol (c)*; **4**, 1321-1324, 2007

S.3. Corradi G, Watterich A, Polgár K, Nagirnyi* V, Hofstaetter* A, Rakitina* LG, Meyer* M; EPR of Cu^{2+} in lithium tetraborate single crystals; *phys stat sol (c)*; **4**, 1276-1279, 2007

S.4. Nagirnyi* V, Kotlov* A, Corradi G, Watterich A, Kirm* M; Electronic transitions in $Li_2B_4O_7$:Cu single crystals; *phys stat sol (c)*; **4**, 885-888, 2007

S.5. Lengyel K, Kovács L, Péter Á, Polgár K, Corradi G, Bourson* P; The effect of Mg doping on the Raman spectra of $LiNbO_3$ crystals; *phys stat sol (c)*; **4**, 847-850, 2007

S.6. Kovács L, Péter Á, Ivleva* LI, Baraldi* A, Capelletti* R; Hydroxil ions in scheelite type molybdates and tungstates; *phys stat sol (c)*; **4**, 856-859, 2007

S.7. Mandula G, Ellabban* MA, Fally* M; A method to determine H^+ concentration in dehydrated iron doped lithium niobate using photorefractive beam fanning effect; *Ferroelectrics*; **352**, 118-124, 2007

S.8. Gruber* JB, Sardar* DK, Yow* RM, Valiev* UV, Mukhammadiev* AK, Sokolov* VY, Amin* I, Lengyel K, Kachur* IS, Piryatinska* VG, Zandi* B; Analysis of the optical and magneto-optical spectra of $Tb_3Ga_5O_{12}$; *J Appl Phys*; **101**, 023108/1-14, 2007

S.9. Araujo* RM, Lengyel K, Jackson* RA, Kovács L, Valerio* MEG; A computational study of intrinsic and extrinsic defects in $LiNbO_3$; *J Phys: Condens Matter*; **19**, 046211/1-10, 2007

S.10. Lengyel K, Kovács L, Péter Á, Polgár K, Corradi G; The effect of stoichiometry and Mg doping on the Raman spectra of $LiNbO_3$:Mg crystals; *Appl Phys B*; **87**, 317-322, 2007

S.11. Berneschi* S, Conti* GN, Bányász I, Watterich A, Khanh* NQ, Fried* M, Pászti* F, Brenci* M, Pelli* S, Righini* GC; Ion beam irradiated channel waveguides in Er^{3+}-doped tellurite glass; *Appl Phys Lett*; **90**, 121136/1-3, 2007

S.12. Kovács L, Capelletti* R, Gospodinov* M; Vibrational frequencies of the impurity-centred oxygen tetrahedra in sillenites; *Vibrational Spectroscopy*; accepted for publication; available online, DOI:10.1016/j.vibspec.2007.10.004

S.13. 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 letters*; accepted for publication

S.14. 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 letters*; accepted for publication

S.15. 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*; accepted for publication

Article in Hungarian

S.16. Hartmann E; Bíró Gábor (1925-2007) (Gábor Bíró, in Hungarian); *Fizikai Szemle*; **57,** 162-163, 2007

Conference proceedings

S.17. Bányász I, Mandula G; Quasi in-situ microscopic study of hologram build-up in $LiNbO_3$ crystals; In: *Practical Holography XXI: Materials and Applications, San Jose, CA, USA, January 19-25, 2007,* Eds.: R. A. Lessard, H. I. Bjelkhagen, Proceedings of SPIE, Bellingham, WA, USA, **6488;** pp. 648808/1-10, 2007

S.18. Berneschi S*, Brenci* M, Conti* GN, Pelli* S, Righini* GC, Bányász I, Watterich A, Khanh* NQ, Fried* M, Pászti* F; Channel waveguides fabrication in Er^{3+}-doped tellurite glass by ion beam irradiation; In*: Integrated Optics: Devices, Materials, and Technologies XI*, *San Jose, CA, USA, January 19-25, 2007,* Eds.: Y. Sidorin, C. A. Waechter, Proceedings of SPIE, Bellingham, WA, USA, **6475**; pp. 647509/1-6, 2007

See also: R.1., R.4., R.8., R.10., R.11., R.17.

T. NONLINEAR AND QUANTUM OPTICS

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, A. Vukics

Laser-induced dynamics of atoms, cavity QED. — The effect of the dipole-dipole interaction on the far-off-resonance optical dipole trapping scheme was calculated by a mean-field approach. The trapping laser field polarizes the atoms and the accompanying dipole-dipole energy shift deepens the attractive potential minimum in a pancake-shaped cloud. At high density the thermal motion cannot stabilize the gas against self-contraction and an instability occurs. We calculated the boundary of the stable and unstable equilibrium regions on a two-dimensional phase diagram of the atom number and the ratio of the trap depth to the temperature. We discussed the limitations imposed by the dipole-dipole instability on the parameters needed to reach Bose-Einstein condensation in an optical dipole trap.

We have investigated the dynamics of 1-dimensional optical lattices in the strong collective coupling regime of light-matter interaction. Using the transfer matrix method, we have taken scattering of the lattice light by the trapped particles into account to all orders. For asymmetric pumping, we have found that traveling density waves arise in the lattice, which can ultimately destabilize it, even in the overdamped limit. This shows explicitly that in this regime the dynamics cannot be described in terms of an "optical potential", an approach often encountered in the literature. We have discussed the shortcomings of the potential energy approach, and shown different derivations of the optical force, in this 1-dimensional model. We have fully characterized the traveling density waves analytically and numerically.

Laser-illuminated atoms in an optical resonator exhibit a phase transition between the homogenous distribution and two possible ordered configurations in the optical lattice formed by the cavity and pump fields. At zero temperature, atom-field entanglement plays a crucial role in the spatial reordering of the atoms from a homogeneous towards the two ordered states, where all atoms occupy either only even or only odd lattice sites. Concurrent with the buildup of atom-field entanglement, the homogeneous atomic cloud evolves immediately into the superposition of the two stable patterns entangled with opposite cavity field amplitudes. This possibility is absent in a factorized (classical) treatment of atoms and field and should be generic for spontaneous symmetry breaking in quantum phase transitions in optical potentials.

Quantum information, entanglement and teleportation. — We have analyzed the realization of a quantum-walk search algorithm in a passive, linear optical network. We have shown that deviations from directionally uniform photon losses lead to the enhancement of the search efficiency compared to uniform loss with the same average. In certain cases even increasing loss in some of the directions can improve search efficiency. We have shown that while we approach the classical limit of the general search algorithm by introducing random phase fluctuations, its utility for searching is lost. Using numerical methods, we found that for static phase errors the averaged search efficiency displays a damped oscillatory behaviour that asymptotically tends to a non-zero value.

The rapid development of quantum control makes it now possible to create large scale quantum entanglement in various physical systems, e.g., in trapped ions or cold atoms. Since full quantum tomography in these cases is not possible, for the detection of

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entanglement one has to find methods that need few measurements. Moreover, in many-particle systems typically the particles cannot be addressed individually. Thus these methods can only use collective measurements. We have been working on methods for entanglement detection under these circumstances. On the one hand, we participated in an experiment carried out at the Max Planck Institute for Quantum Optics, where a four-qubit quantum state was created with photons, and the methods developed were used for entanglement detection. On the other hand, we determined the complete set of generalized spin squeezing inequalities that can detect entanglement in many-particle experiments. Finally, we worked on other aspects of entanglement detection issues related to mixed state quantum computing, and local hidden variable models.

We generalized the concept of recurrence probability (Pólya number) for d-dimensional unbiased quantum walks. A sufficient condition for a quantum walk to be recurrent was derived. As a by-product we have found a simple criterion for localisation of quantum walks. In contrast to classical walks, where the Pólya number is characteristic for the given dimension, the recurrence probability of a quantum walk depends in general on the topology of the walk, choice of the coin and the initial state. This allows to change the character of the quantum walk from recurrent to transient by altering the initial state.

Nuclear motion in molecules. — dynamics and spectroscopy. – A technique has been developed which in principle allows the determination of the full rotational-vibrational eigenspectrum of triatomic molecules by treating the important singularities present in the triatomic rotational-vibrational kinetic energy operator given in Jacobi coordinates and the R, embedding. A generalized finite basis representation resulting in a nonsymmetric Hamiltonian matrix has been employed. The basis set to be used is obtained by taking the direct product of a 1-D DVR basis, related to R1, with a 5-D nondirect-product basis, the latter formed by coupling Bessel-DVR functions depending on the distance-type coordinate causing the singularity, associated Legendre polynomials depending on the Jacobi angle, and rotational functions depending on the three Euler angles. The robust implicitly restarted Arnoldi method within the ARPACK package is used for the determination of a number of eigenvalues of the nonsymmetric Hamiltonian matrix. The suitability of the proposed approach is shown by the determination of the rotational-vibrational energy levels of the ground electronic state of H-3(+) somewhat above its barrier to linearity. Convergence of the eigenenergies is checked by an alternative approach, employing a Hamiltonian expressed in Radau coordinates, a standard direct-product basis, and no treatment of the singularities.

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Grants and international cooperations

OTKA T049234 Quantum optical systems and applications in quantum informatics (J. Janszky, 2005-2008)
OTKA T043079 Moving atoms and molecules in strongly-coupled radiation fields (P. Domokos, 2003-2007)
OTKA NF68736 Cavity Quantum Electrodynamics of systems from few atoms to controlled ensembles (P. Domokos, 2007-2010)
OTKA T045955 Theoretical methods to describe vibrational-rotational motion of molecules (V. Szalay, 2004-2007)
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, 2006-2007)
TéT, Hungarian-Spanish Bilateral Intergovernmental S&T Cooperation (ESP-17/2006): Quantum control (V. Szalay, 2007-2008)
FP6 Marie Curie European Reintegration Grant of the European Commission (MERG-CT-2005-029146): Detection of multipartite entanglement in quantum optical systems (G. Tóth, 2006-2007)
Öveges József program: Qubit dynamics in quantum optical networks (T. Kiss, 2006-2007)
Öveges József program: Cavity Quantum Electrodynamics: from atoms to many-body systems (P. Domokos, 2006-2007)

Publications

Articles

T.1. Gühne* O, Mechler* M, Tóth G, Adam P; Entanglement criteria based on local uncertainty relations are strictly stronger than the computable cross norm criterion; *Phys Rev A*; **74**, 010301/1-4, 2006

T.2. Kiss T, Jex* I, Alber* G, Vymetal* S; Complex chaos in conditional qubit dynamics and purification; *Acta Phys Hung B*; **26**, 229–235, 2006

T.3. Kurucz Z, Ádám P, Janszky J; Remote state preparation in quadrature basis; *Acta Phys Hung B*; **26**, 319-326, 2006

T.4. Nagy D, Asbóth J, Domokos P; Collective cooling of atoms in a ring cavity; *Acta Phys Hung B*; **26**, 141-148, 2006

T.5. Stefanak* M, Kiss T, Jex* I, Mohring* B; The meeting problem in the quantum walk; *J Phys A*; **39**, 14965-14983, 2006

T.6. Almeida* ML, Pironio* S, Barrett* J, Tóth G, Acín* A; Noise robustness of the nonlocality of entangled quantum states; *Phys Rev Lett*; **99**, 040403/1-4, 2007

T.7. Asbóth JK, Domokos P; Comment on "Coupled dynamics of atoms and radiation-pressure-driven interferometers" and "Superstrong coupling regime of cavity quantum electrodynamics"; *Phys Rev A*; **76**, 057801/1-4, 2007

T.8. Asbóth JK, Ritsch* H, Domokos P; Collective excitations and instability of an optical lattice due to unbalanced pumping; *Phys Rev Lett*; **98**, 203008/1-4, 2007

T.9. Czakó* G, Császár* AG, Szalay V, Sutcliffe* BT; Adiabatic Jacobi corrections for H-2(+)-like systems; *J Chem Phys*; **126**, 024102/1-10, 2007

T.10. Czakó* G, Furtenbacher* T, Barletta* P, Császár* AG, Szalay V, Sutcliffe* BT; Use of a nondirect-product basis for treating singularities in triatomic rotational-vibrational calculations; *Phys Chem Chem Phys*; **9**, 3407-3415, 2007

T.11. Gabris A, Agarwal* GS; Quantum teleportation with pair-coherent states; *Int J Quant Inf*; **5**, 17-22, 2007

T.12. Kiesel* N, Schmid* C, Tóth G, Solano* E, Weinfurter* H; Experimental observation of four-photon entangled Dicke state with high fidelity; *Phys Rev Lett*; **98**, 063604/1-4, 2007

T.13. Maes* C, Asbóth JK, Ritsch* H; Self ordering threshold and superradiant backscattering to slow a fast gas beam in a ring cavity with counter propagating pump; *Optics Express*; **15**, 6019-6035, 2007

T.14. Maschler* C, Ritsch* H, Vukics A, Domokos P; Entanglement assisted fast reordering of atoms in an optical lattice within a cavity at T = 0; *Opt Communications*; **273**, 446-450, 2007

T.15. Nagy D, Domokos P; Dipole-dipole instability of atom clouds in a far-detuned optical dipole trap; *Phys Rev A*; **75**, 053416/1-8, 2007

T.16. Tóth G, García-Ripoll* JJ; Efficient algorithm for multi-qudit twirling; *Phys Rev A*; **75**, 042311/1-11, 2007

T.17. Tóth G; Detection of multipartite entanglement in the vicinity of symmetric Dicke states; *J Opt Soc Am B*; **24**, 275-282, 2007

T.18. Vasilopoulos* P, Kalman O, Peeters* FM, Benedict* MG; Aharonov-Bohm oscillations in a mesoscopic ring with asymmetric arm-dependent injection; *Phys Rev B*; **75**, 035304/1-7, 2007

T.19. Szirmai G, Domokos P; Geometric resonance cooling of polarizable particles in an optical waveguide; *Phys Rev Lett*; **99**, 213602/1-4, 2007

T.20. Gabris A, Kiss T, Jex* I; Scattering quantum random-walk search with errors; *Phys Rev A*; accepted for publication

T.21. Kalman O, Foldi* P, Benedict* MG, Peeters* FM; Spatial interference induced spin polarization in a three-terminal quantum ring; *Physica E*; accepted for publication

T.22. Stefanak* M, Jex* I, Kiss T; Recurrence and Pólya number of quantum walks; *Phys Rev Lett*; accepted for publication.

T.23. Tóth G, Knapp* C, Gühne* O, Briegel* HJ; Optimal spin squeezing inequalities detect bound entanglement in spin models; *Phys Rev Lett*; accepted for publication; quant-ph/0702219.

Conference proceeding

T.24. Schmid* C, Kiesel* N, Laskowski* W, Solano* E, Tóth G, Zukowski* M, Weinfurter* H; The Entanglement of the Symmetric Four-Photon Dicke State; In: *Quantum Communication and Security, Proceedings of the NATO Advanced Research Workshop on Quantum Communication and Security, Gdansk, Poland, 10-13 Sept. 2006*; Eds.: M. Zukowski, S. Kilin, and J. Kowalik, IOS Press (ISBN 978-1-58603-749-9), Netherlands; p. 113, 2007

See also B.3.

EDUCATION

Graduate and postgraduate courses, 2007

— Completely integrable many body systems (F. Woynarovich, ELTE[1])

— Advanced solid-state physics (J. Sólyom ELTE)

— Electrodynamics of continuos media (F. Woynarovich, ELTE)

— Statistical physics (F. Iglói , SZTE[2])

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

— Disordered systems (F. Iglói, SZTE)

— Many body systems I. (P. Szépfalusy, ELTE)

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

— The theory of magnetism I (P. Fazekas, BME[3])

— Metal physics (J. Kollár, BME)

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

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

— Amorphous and crystalline materials (regular lecture for 4th grade engineering physics students) (S. Kugler* and T. Kemény, BME)

— Calorimetry (in the framework of "Experimental methods in solid state research" course, 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, BME and ELTE)

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

— Superconductivity (G. Kriza, BME)

— Application of thermal neutrons for study of condensed matter (L. Cser, ELTE)

[1] ELTE = Loránd Eötvös University, Budapest

[2] SZTE = University of Szeged

[3] BME = Budapest University of Technology and Economics

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

— Neutron scattering in condensed matter (L. Rosta, ME[4])

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

— From femtosecond lasers to attophysics (P. Dombi, SZTE[5])

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

— Growth, processing and characterization of nonlinear optical crystals (In: Applied Lasertechnics, 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)

— Thermodynamics (P. Ádám, PTE[6])

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

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

— Open Quantum Systems (P. Ádám, PTE)

— Theory of laser cooling and trapping (P. Domokos, ELTE, BME)

— Quantum mechanics (J. Janszky, PTE)

— Quantum information theory (P. Ádám, PTE)

— Applied optics (T. Kiss, ELTE)

— Information theory (M. Koniorczyk, PTE)

— Many-body problem in quantum mechanics (M. Koniorczyk, PTE)

— Introduction to programming (M. Koniorczyk, PTE)

— Operating systems II. (M. Koniorczyk, PTE)

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

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

— Many-body problems I. (G. Szirmai, P. Szépfalusy, ELTE)

— Many-body problems II. (P. Szépfalusy, G. Szirmai, ELTE)

[4] ME = University of Miskolc

[5] SZTE = University of Szeged

[6] PTE = University of Pécs

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)

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

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

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

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

— NMR spectroscopy (K. Tompa, BME)

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

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

— Experimental physics laboratory course (Sz. Pothoczki, BME)

— 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)

— Introduction to statistical physics (J. Asboth, PTE)

— Quantum mechanics (J. Janszky, PTE)

Diploma works

V. Poór (ELTE): Electrodeposition of metals from ionic liquids (Supervisor: L. Péter)

E. Simon (ELTE): Study of giant magnetoresistance and coupling in Co-Cu/Cu multilayers (Supervisor: I. Bakonyi)

C. Schimpf (Technische Universität Bergakademie Freiberg, Germany): Microstructure and magnetoresistance of Co/Cu multilayers deposited using electrochemical deposition (Co-supervisor: I. Bakonyi)

Ph. D. students

K. Buchta (ELTE): Phase transitions in low-dimensional spin and fermionic models (Supervisor: J. Sólyom)

K. Németh (ELTE): Chemical functionalization of carbon nanotubes (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 filed modeling of microstructures (Supervisor: L. Gránásy)

G. 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)

L. Németh (BME): NMR study of low-dimensional metals (Supervisor: G. Kriza)

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

M. Markó (BME): Neutron holography (Supervisor: L. Cser)

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

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)

J. Orbán (BME): Study and developing of readout electronic of position sensitive neutron detectors (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)

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)

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

J. Asbóth (SZTE): Atom-atom interactions mediated by optical resonator fields (Supervisor: P. Domokos)

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

Dissertations

G. Oszlányi: Crystal structure of C_{60} polimers (D.Sc., Hungarian Academy of Sciences)

I. Bakonyi: Electronic structure and magnetic properties of Ni-based metastable alloys (D.Sc., Hungarian Academy of Sciences)

P. Domokos: Mechanical effects of light on atoms in optical resonators (D. Sc., Hungarian Academy of Sciences)

E. Szirmai: Mott transition in SU(*n*) symmetric Hubbard chains and ladders (PhD, ELTE, supervisor: J. Sólyom)

F. Borondics: Optical studies and functionalization of single-walled carbon nanotubes (PhD, ELTE, supervisor: K. Kamarás)

É. Kováts: Topochemical reactions of crystalline fullerene derivatives (PhD, ELTE, supervisor: S. Pekker)

P. Matus: Influence of C_{60} local orientation on electronic properties of A_3C_{60} compounds (Ph.D, BME, Supervisor: G. Kriza)

L. Temleitner: Investigation of structural disorder by neutron diffraction and computer simulation (Ph.D, BME, Supervisor: L. Pusztai)

P. Horváth: Mass spectroscopic and optical studies of radiofrequency SiH_4 and H_2-SiH_4 plasmas (PhD, ELTE, Supervisor: K. Rózsa, A. Gallagher*)

G. Czakó: Quantum chemical calculation of the full spectra of small molecules (Ph.D., ELTE, Supervisor: V. Szalay)

A. Gábris: Multipartite quantum optical systems for quantum information processing (Ph.D., SZTE, Supervisor: J. Janszky)

Z. Kurucz: Entanglement assisted quantum communication schemes (Ph.D., SZTE, Supervisor: J. Janszky)

AWARDS

— K. Tompa: József Eötvös Laureate (HAS, 2007)

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

— L. Kőszegi: Pál Selényi Award of the Loránd Eötvös Physical Society

— P. Hartmann, V. Zólyomi: Young Scientist Award of the HAS (2007)

— F. Borondics: SZFKI Annual Publication Award (2007)

— P. Kamasa: SZFKI Annual Award for Applied Research (2007)

— M. Koniorczyk: Award of the Committee of the Hungarian Acedemy of Sciences in Pécs

— V. Poór (ELTE): Diploma Work Excellence Award 2007, Hungarian Chemical Society (Supervisor: L. Péter)

— G. Nagy: Young Scientist Award of ENSA (European Neutron Scattering Association), ECNS07, Lund conference, June 2007

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

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

— P. Dombi: Bolyai Grant (2007-2010)

— M. Veres, Bolyai Grant (2006-2008)

— L. Péter, Bolyai Grant (2004-2006)

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)

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

— 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

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

— K. Fodor-Csorba: Member of the International Liquid Crystal Society, Board of Directors

— 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)

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

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

— 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: Europhyics Conference on Atomic and Molecular Physics in Ionized Gases (ESCAMPIG)

— Z. Donkó: Member of the International Scientific Committee of conference series: Symposium on the Physics in Ionized Gases (SPIG)

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

— A. Czitrovszky: Member of the Board 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: 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. Kovács: Member of the International Advisory Committee, Europhysical Conferences on Defects in Insulating Materials

— L. Kovács: Member of the Programme Committee, International Conference on Defects in Insulating Materials 2008, Brazil

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

— P. Domokos: Editor of the European Physical Journal D

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

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

CONFERENCES

— **Electrochemistry seminar** (Budapest, Hungary, Oct. 15-19, 2007). Within the framework of a bilateral Science and Technology Collaboration project (Romania-Hungary, TéT RO-22/05), L. Péter and I. Bakonyi organized a seminar on basic issues of electrochemistry with particular reference to the electrodeposition of metals, alloys and multilayers from aqueous solutions which is the main topic of the collaborative bilateral project. Within the seminar program, L. Péter gave 8 tutorial lectures on electrochemistry and elctrodeposition of metallic materials and I. Bakonyi gave one lecture on atomistic aspects of nucleation and growth during deposition from solution and from the vapour phase. Altogether about 10 scientists and students participated

— **Hungarian-Indian Bilateral Workshop on Condensed Matter Research**: Magnetic Materials (University of Hyderabad, India, Dec. 4, 2006). On the occasion of the Silver Jubilee (25 years) of collaboration between HAS and INSA (Indian national Science Academy), a one-day workshop was organized in Hyderabad by S.N. Kaul (University of Hyderabad) and I. Bakonyi (RISSPO HAS). In the scientific program of the workshop, 3 scientists of RISSPO HAS and 4 Indian scientists (two from Hyderabad and two from other leading Indian research institutes) presented lectures on magnetic and magnetotransport properties of materials which are in the forefront of current research interest worldwide, including e.g., magnetic nanostructures. The workshop was attended by some 50 scientists among them with a group of Ph.D. students from all over India who participated in a usual annual lecture course series on solid state physics in Hyderabad just that week. A poster session was also held during the workshop.

— The **4th Central European Training School on Neutron Scattering** (**CETS'2007)** organized by the Neutron Spectroscopy Department was held in Budapest from April 23-28, 2007. The scope of this course was to provide insight into neutron scattering techniques and their application for studies on structure and dynamics of condensed matter. This training opportunity was offered to the European community with special emphasis on the Central European region and with a special regard on neutron optics. The 18 hours of lectures given by scientists from the leading European neutron centers (ILL-Grenoble, HMI-Berlin, LLB-Saclay, JINR-Dubna, NPI-Prague, BNC-Budapest, University of Vienna) gave an introduction on neutron scattering techniques; the experiments on neutron spectrometers have demonstrated to the students the art of utilization of instruments at a large scale facility. Experiments on the following machines were performed: small-angle neutron scattering instrument, three-axis spectrometer, neutron reflectometer (multilayer reflectivity), prompt-gamma activation analysis, data imaging and analysis of anisotropic scattering spectra. The school provided a forum for the presentation and discussion of actual research works of young scientists in the course of a half-day program, which was devoted to a poster/short oral presentation session. The participants (32 students) were young physicists, chemists, biologists, and actual or potential neutron users from the different countries of Europe (Austria, Bulgaria, Czech Republic, Finland, Hungary, Italy, Romania, Russia, Ukraine).

— A joint **Workshop on Neutron Instrumentation** was held in on October 25-27 in Budapest, devoted to the modernisation and instrument development programme of the 8 MW reactor of the Kurchatov Institute (Moscow). The meeting organized by the Research Institute for Solid State Physics and Optics and the Russian Centre

“Kurchatov Institute” with 20 participants made and overview of the instrument suite at BNC and the modernisation project in Moscow.

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