ANNUAL REPORT

2002

RESEARCH INSTITUTE FOR SOLID STATE PHYSICS AND OPTICS

of the Hungarian Academy of Sciences, Budapest, Hungary

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2002

Host institute of the KFKI Condensed Matter Research Centre

CENTRE OF EXCELLENCE

RESEARCH INSTITUTE FOR SOLID STATE PHYSICS AND OPTICS

of the Hungarian Academy of Sciences, Budapest, Hungary

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ANNUAL REPORT 2002

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Dear Reader,

It is my pleasure to hand over the Annual Report of the Research Institute for Solid State Physics and Optics in 2002.

Our institute was founded by the Hungarian Academy of Sciences in 1981 as part of the Central Research Institute for Physics. In 1992 we became an independent institute and along with our status changed our name as well: "Research Institute for Solid State Physics". In 1998 the Crystal Physics Laboratory of the Hungarian Academy of Sciences joined our institute as a part of the reorganisation process of the academic institutes and at the same time our name has been altered to "Research Institute for Solid State Physics and Optics".

The main profile of the institute is basic research in the fields of theoretical and experimental solid state physics and materials science including metal physics, crystal physics and liquid crystal research, theoretical and experimental optics including laser physics, quantum optics and the interaction of light with matter. Our experimental research activity is connected to unique methodologies like X-ray diffraction, NMR-, Mössbauer-, and optical spectroscopy and neutron scattering experiments at the KFKI Research Reactor. Some of our research (R & D) activities are more closely related to applications, first of all in the fields of optical thin films, laser applications, crystal growing technologies and metallurgy.

Our research activity is financed by the Hungarian Academy of Sciences and by national and international research funds like the Hungarian National Research Fund (OTKA) and also through individual projects. Since Hungary has joined the EU 5th Framework Programme, the international co-operation has become even more important for the scientific work of our research groups. Our institute, as the host of the KFKI-Condensed Matter Research Centre (CMRC) is taking part in the "*Centre of Excellence" programme of the European Union.* We are involved in several international projects in collaboration with a great number of research institutions and universities. More than half of our publications (about 60 percent) feature foreign co-authors, indicating the significant role of these partnerships. The different EU, ESF, COST, NATO and other international projects play a rapidly increasing role in our research activity. The share of these international resources in our budget is nearly 10% (EU funds in 2001 were 13%; in 2002 8% of our budget). A remarkable increase can be observed concerning investments, which is very appealing taking into account the average age of our equipment. We are participating in three projects of the National Research and Development Program (NKFP); two is concerning nanotechnology, while the third is concentrating on the study of environmental pollution caused by atmospheric aerosols.

Our institute has a long tradition in graduate and to a larger extent in post-graduate education. Details of this activity are also given in this Annual Report. We have published more than 200 papers in high quality international journals and conference proceedings. The number of these publications is similar to that of the previous years. In 2002 two of our scientists have become Doctors of the Hungarian Academy of Sciences (DSc).

I hope that this booklet gives 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 WEB page at www.szfki.hu

B u d a p e s t, 29 November, 2017

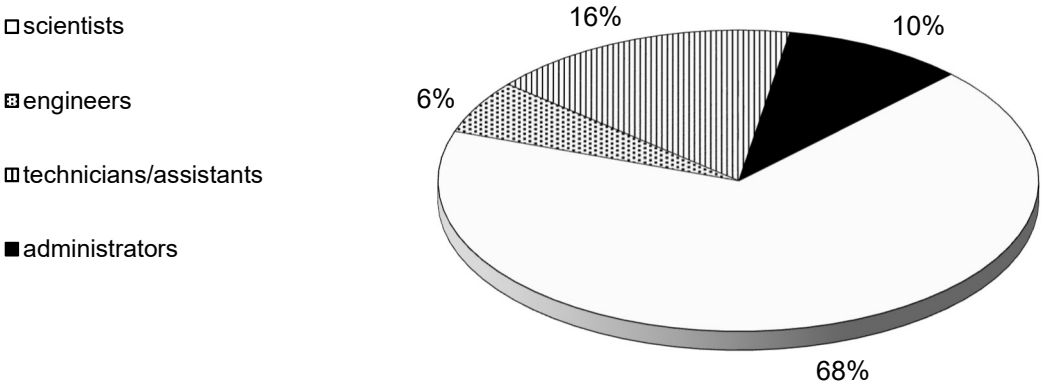
János Kollár

Director

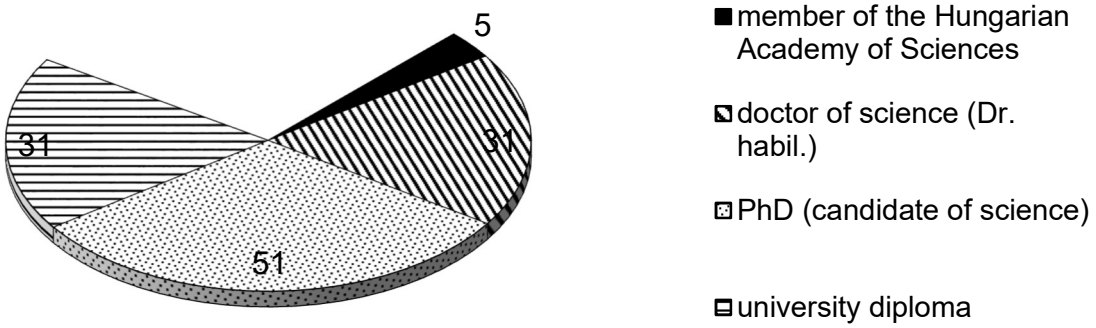
Key figures

Permanent staff of the Institute: 170 employees. Its distribution:

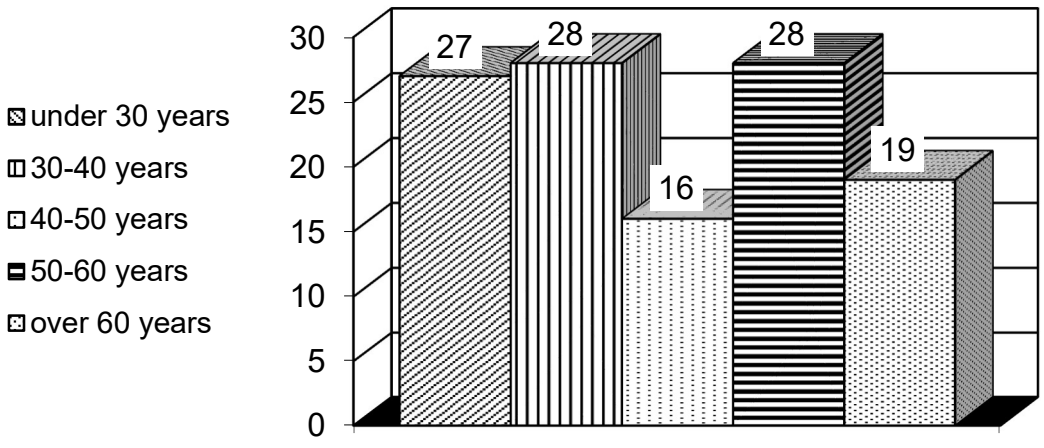
a) by professions:



b) by scientific titles/degrees:

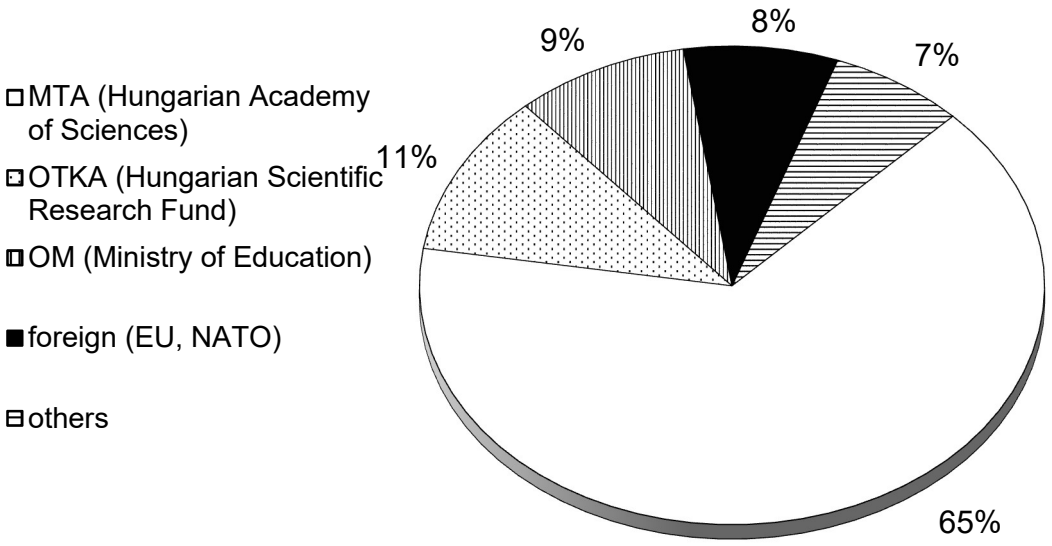


c) by ages:

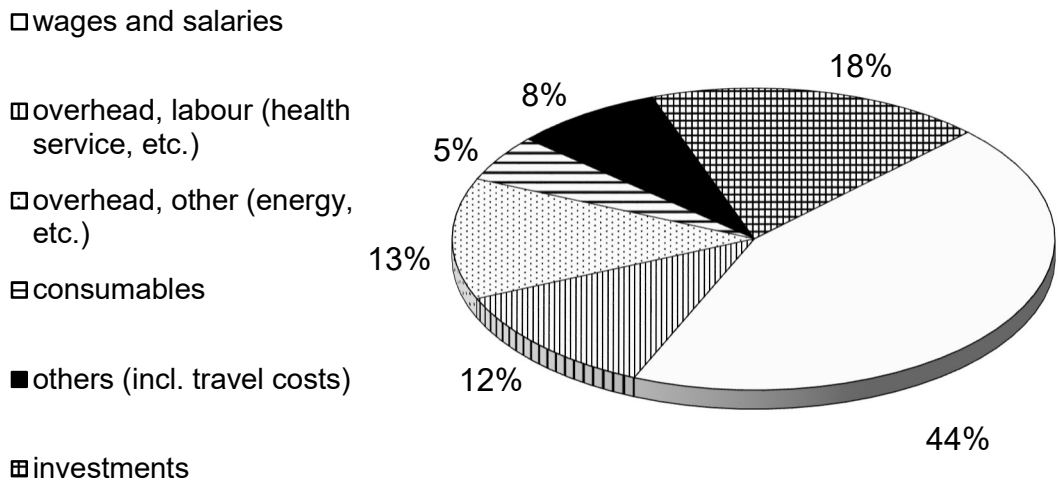


Financial management

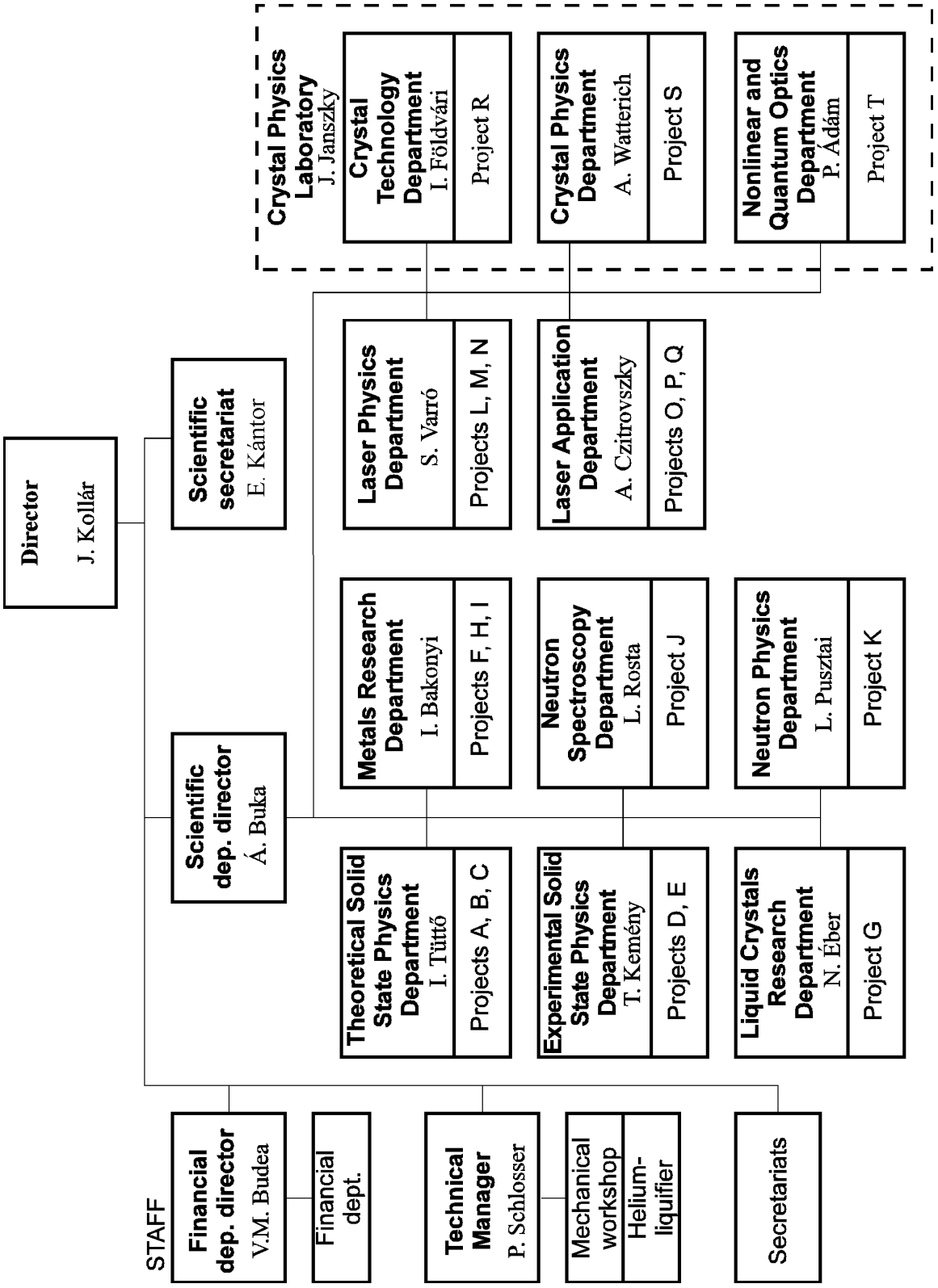
a) Sources of operation costs:



b) Distribution of expenditures:



Structure of the Research Institute for Solid State Physics and Optics



A. STRONGLY CORRELATED SYSTEMS

J. Sólyom, G. Fáth, E. Kiss[#], *Ö. Legeza, K. Penc, K. Vladár, F. Woynarovich, A. Zawadowski*[+]

Low dimensional magnetic models. — Antiferromagnetic Heisenberg spin chains in a sufficiently strong magnetic field are Luttinger liquids, whose parameters depend on the actual magnetization of the chain. We computed precise numerical estimates of the Luttinger liquid dressed charge Z, which determines the critical exponents, by calculating the magnetization and quadrupole operator profiles for S=1/2 and S=1 chains using the density matrix renormalization group method. Critical amplitudes and the scattering length at the chain ends are also determined. Although both systems are Luttinger liquids the characteristic parameters were found to differ considerably.

Fermionic and bosonic models. — We have studied the relationship between the real error and truncation error of the Density Matrix Renormalization Group (DMRG) method in momentum space (k-DMRG). We have showed numerically that it is possible to determine the desired accuracy of the method in advance of the calculations by dynamically controlling the truncation error and the number of block states using a novel protocol which we dubbed Dynamical Block State Selection (DBSS).

We have also studied the ionic-neutral curve crossing between the two lowest $^1\Sigma^+$ states of LiF in order to demonstrate the efficiency of the quantum chemistry version of the density matrix renormalization group method (QC-DMRG). We have calculated the ground and several low-lying excited state energies and the dipole moment as a function of bond length, which in fact provided a smooth and continuous curve even close to the avoided crossing, in contrast to other standard numerical treatments.

We have developed a new *infinite lattice* method applicable within the framework of the k-DMRG and studied the one dimensional Hubbard model for weak- and strong-coupling limit. In addition to the ground and low lying excited state energies we have also calculated the one particle momentum distribution function, which agreed very well with the analytic formula of Koch and Goedecker in the strong coupling limit.

We studied the thermodynamics of surface states, in Bethe Ansatz solvable systems. In one dimensional systems the surface states give ordo one contribution to the free energy. For this reason it is important to know the bulk free energy up to this accuracy. We have developed a method to calculate the ordo one contributions of the saddle-point fluctuations to the free energy of Bethe Ansatz systems.

We have studied the exact one-electron propagator and spectral function of a solvable model of electrons interacting due to a gauge coupling. For the model not only the energies, but the wave functions are also found exactly, thus allowing us to calculate the spectral functions that turn out to be interesting, and nontrivial. They provide one of the few examples of cases where the spectral functions are known asymptotically as well as exactly.

Kondo problem. — Two examples of two level systems were studied where breaking of the electron-hole symmetry leads to instabilities of scaling trajectories. The actual infrared cutoff (which depends on the asymmetry, too) doesn't allow to reach the new fixed point but

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

the electron-hole asymmetry can result enhancement of the effective couplings and the Kondo temperature.

Other problems. — We investigated pricing and buyer/seller adoption dynamics problems in a stochastic model of an electronic exchange. We demonstrated that an anomalously slow (fat-tail) decay of the consumer-product fit distribution function would lead to the increase of the equilibrium price as buyer-seller connectivity increases. This result is counter-intuitive as it means that prices increase albeit supplier competition becomes stronger. As for the adoption dynamics, we identified two stable fixed points (low- and high participation), and showed that the two are separated by a saddle point. The saddle point defines a critical mass line (separatrix) for the exchange.

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Alfréd Zawadowski	zawa@phy.bme.hu

Grants

OTKA[1] T 030173 Theoretical study of magnetically or electrically low-dimensional models (J. Sólyom, 1999-2002)

OTKA F031949 Effect of magnetic field on the behavior of quantum spin chains (G. Fáth, 2000-2003)

OTKA F 032231 Study of coupled spin and fermion chains with the density matrix renormalization method (Ö. Legeza, 2000-2003)

OTKA D32689 (postdoctoral). Spin and orbital ordering in frustrated vanadium oxydes and sulphides (K. Pencz, 2001-2002)

Long term visitors:

— Anja Grage, Marburg University (September 2002 - February 2003)

— Holger Benthien, Marburg University (September 2002 - February 2003)

Publications

Articles

A.1. Penc K, Shastry* BS; Exact spectral functions of a non-Fermi liquid in one dimension; *Phys Rev B*; **65**, 155110/1-7, (2002)

A.2. Újsághy* O, Vladár K, Zaránd* G, Zawadowski A; The role of electron-hole symmetry breaking in the Kondo problems; *Journal of Low Temperature Physics*; **126**, 1221-1231, (2002)

[1] OTKA - Hungarian Research Fund

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

A.3. Fáth G; Luttinger liquid behavior in spin chains with magnetic field; *Phys. Rev. B*; accepted for publication

A.4. Legeza Ö, Röder* J, Hess* BA; QC-DMRG study of the ionic-neutral curve crossing of LiF; *J. Mol. Chem.*; accepted for publication; cond-mat: 0208187

A.5. Fáth G, Sarvary* M; Adoption dynamics in buyer-side exchanges; *Quantitative Marketing and Economics*; accepted for publication

A.6. Legeza Ö, Röder* J, Hess* BA; Controlling the accuracy of the Density matrix renormalization group method: The Dynamic Block State Selection approach; *Phys Rev; B*; accepted for publication; cond-mat: 0204602;

Book

A.7. Sólyom J; *A modern szilárdtestfizika alapjai, I. kötet, A szilárd testek szerkezete és dinamikája (Modern solid state physics, Part I, Structure and dynamics of solids, in Hungarian)*; ELTE Eötvös Kiadó; 2002

See also C.14.

B. COMPLEX SYSTEMS

F. Iglói, R. Juhász[#], N. Menyhárd, A. Sütő, P. Szépfalusy

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

Phase transitions and critical behaviour. — Critical properties of quantum spin chains with varying degrees of disorder are studied at zero temperature by analytical and extensive density matrix renormalization methods. Generally the phase diagram is found to contain three phases. The weak disorder regime, where the critical behavior is controlled by the fixed points of the pure system and the strong disorder regime, which is attracted by an infinite randomness fixed point, are separated by an intermediate disorder regime, where dynamical scaling is anisotropic and the static and dynamical exponents are disorder dependent.

We studied first- and second-order phase transitions of ferromagnetic lattice models on scale-free networks, with a degree exponent γ. Using the example of the q-state Potts model we derived a general self-consistency relation within the frame of the Weiss molecular-field approximation, which presumably leads to exact critical singularities. Depending on the value of γ, we have found three different regimes of the phase diagram. As a general trend first-order transitions soften with decreasing γ and the critical singularities at the second-order transitions are γ-dependent.

We have investigated universality classes of continuous phase transitions to absorbing states in (1+1)-dimensional reaction-diffusion systems by carrying out large-scale simulations.

Kinetic Ising models in a locally spin-anisotropic environment have been introduced to study the effect of locally broken spin-symmetry on the dynamic and static critical properties in one dimension. The mostly numerical results indicate a drastic change in the phase diagram and critical behavior.

Quantum systems. — For the free Bose gas we proved that the Bose-Einstein condensation occurs simultaneously with the appearance of macroscopic permutational cycles.

We investigated systems of bosons interacting via contact (point) interactions. In continuous space there are such systems only in 1,2 and 3 dimensions, while on lattices they exist in any dimension. We described a family of exact eigenstates: those eigenstates of the kinetic energy operator vanishing at particle encounters.

We have treated the dynamics of various phase transitions and that of the arising ordered phase. Our main aim was to determine the energy and damping of the elementary excitations in different systems. We have shown that in Bose-condensed spin-1 gases the lifetime of the spin waves is longer than that of the density waves. In the O(n)- symmetric field-theoretical model the detailed theory of the threshold enhancement has been worked out on the basis of the temperature dependence of the properties of the particles.

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Péter Szépfalusy psz@galahad.elte.hu

Grants and international cooperations

OTKA T029552 Study of atomic systems (P. Szépfalusy, 1999-2002)
OTKA T030543 Mathematical study of systems of quantum spins and particles (A. Sütő, 1999-2002)
OTKA T034183 Disordered quantum spin systems (F. Iglói, 2001-2004)
OTKA T034784 Scaling behavior and universality in non-equilibrium systems (N. Menyhárd, 2001-2002)
ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP7: Condensed matter theory (F. Iglói, 2000-2003)
DAAD-MÖB 257/2002 Statistical Physics of Disordered Systems (F. Iglói, 2002-2003)

Publications

Articles

B.1. Carlon* E, Lajkó* P, Iglói F; Disorder induced cross-over effects at quantum critical points; *Phys. Rev. Lett.*; **87**, 277201/1-4, (2001)

B.2. Igói F; Exact renormalization of the random transverse-field Ising spin chain in the strongly ordered and strongly disordered Griffiths phases; *Phys. Rev. B*; **65**, 064416/1-11, (2002).

B.3. Mélin* R, Lin* Y-C, Lajkó* P, Rieger* H, Iglói F; Strongly disordered spin ladders; *Phys. Rev. B*; **65**, 104415/1-10, (2002)

B.4. Turban* L, Iglói F; Surface induced disorder and aperiodic perturbations at first-order transitions; *Phys. Rev. B*; **66**, 014440/1-10, (2002)

B.5. Anglés d'Auriac* J-Ch, Iglói F, Preissmann* M, Sebő* A; Optimal cooperation and submodularity for computing Potts' partition functions with a large number of states; *J. Phys. A*; **35**, 6973-6983, (2002).

B.6. Iglói F, Turban* L; First- and second-order phase transitions in scale-free networks; *Phys. Rev. E*; **66**, 036140/1-4, (2002).

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B.8. Menyhárd N, Ódor* G; One-dimensional nonequilibrium kinetic Ising models with local spin symmetry breaking: N-component branching annihilating random-walk transition at zero branching rate; *Phys. Rev. E*; **66,** 016127/1-5, (2002)

B.9. Sütő A; Percolation transition in the Bose Gas: Part II; *J. Phys. A: Mat. Gen.*; **35**, 6996-7002, (2002)

B.10. Sütő A; Exact eigenstates for contact interactions; *J. Stat. Phys.*; **109**, 1051-1072, (2002).

B.11. Szépfalusy P, Szirmai* G; Structure of the perturbation series of the spin-1 Bose gas at low temperatures; *Phys. Rev. A*; **65**, 043602/1-25, (2002)

B.12. Szépfalusy P; Properties of permanent and transient chaos in critical states; *Advances in Chemical Physics*; **122**, 49-51, (2002)

B.13. Patkós* A, Szép* Zs, Szépfalusy P; Finite temperature spectral functions of the linear O(n)-model at large-N applied to the π-σ system; *Physics Letters B*; **537**, 77-87, (2002)

B.14. Patkós* A, Szép* Zs, Szépfalusy P; Second sheet σ-pole and the threshold enhancement of the spectral function in the scalar-isoscalar meson - sector; *Phys. Rev. D*; accepted for publication

Conference proceeding

B.15. Patkós* A, Szép* Zs, Szépfalusy P; Finite temperature spectral function of the σ meson from large-N expansion. In: *Proc. Budapest'02 Workshop on Quark & Hadron Dynamics (2002)*, Ed: P. Lévai, EP Systema, Debrecen, Hungary; 243-251, (2002)

C. ELECTRONIC STATES IN SOLIDS

J. Kollár, P. Fazekas, K. Itai, A. Kiss[#], I. Tüttő, B. Újfalussy, A. Virosztek[+] , L. Vitos

Within the framework of the *exact muffin-tin orbitals* (EMTO) theory, and the *coherent potential approximation* (CPA), a new method to calculate the total energy for random substitutional alloys has been developed.

The EMTO-CPA method was used to determine **elastic properties of $Ag_{1-c}Zn_c$** random alloys in the face-centered and body-centered cubic crystallographic phases. The theoretical cubic elastic constants, and the Debye temperatures are in very good agreement with the available experimental results. Rapid variations of cubic shear moduli are observed at high Zn concentrations, which contradicts the common empirical observation that alloying has only minor effects on elastic properties.

In the near past, an atomic level description of **alloy steels**, still seemed to be unattainable. However, the recently developed FCD-EMTO (Full Charge Density-EMTO) method opens unique possibilities in the field of computational alloy steel design. We have employed the FCD-EMTO method in a *quantitative* description of the electronic structure and physical properties of alloy steels. We have established the *elastic property-composition* maps of *austenitic stainless steels*. The so generated data has been used in the search for new steel grades, and as example, two new basic compositions with outstanding properties among the *austenitic stainless steels* have been predicted.

Within the frame of these studies, the high pressure and low temperature **crystal structures of $CaSiO_3$ and $ScAlO_3$ perovskites** have been determined. We proposed a new parametrization method for perovskite structures; we have shown that this method in combination with *ab initio* total energy calculations is suitable to predict changes in the structural distortion under pressure. As a result of these studies we were able to explain the origin of octahedral tilting in orthorhombic perovskite structures.

We studied the **magnetism of small metallic particles** on and in surfaces. The major goal was to develop a first principles based, fully relativistic spin dynamics method able to calculate the ground state, including the orientation of the magnetisation. The sizes of metallic particles ranged from 2 Fe atoms on the surface to quantum corrals of 48 Fe atoms. We found that the magnetisation of two Fe atoms on the surface of Cu(111) is ferromagnetic but it is canted.

We discussed the possible multipolar moments of the f-shells in various Pr compounds, and used the results to construct interaction hamiltonians, and mapped out their phase diagrams. For $PrBa_2Cu_3O_6$ we found that a combination of dipolar and quadropolar interactions acting within the generally assumed Γ_5-like pseudotriplet comes near to accounting for the observed linear and non-linear susceptibilities. For the filled skutterudite $PrFe_4P_{12}$, we have shown that the observed behavior is well modelled with a Γ_1-Γ_4 crystal field scheme. Assuming the presence of antiferroquadrupolar and ferromagnetic dipolar interactions, we calculated the susceptibility, the magnetic field dependence of the specific heat and the magnetization curves, and found good agreement with experiments.

We have continued the exploration of the phase diagram of the correlated transition metal sulphide $BaVS_3$. Using magnetoresistivity measurements, we determined the pressure

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dependence of the spin gap up to 15 kbar. The data indicates that the Mott insulating phase of $BaVS_3$ is characterized by spin-orbital resonance. We analyzed the thermodynamic character of the metal-insulator phase transition, and derived a suitable form of the Ehrenfest-Fisher relation which connects the anomaly of the non-linear magnetic susceptibility with those of the specific heat, and the temperature derivative of the linear susceptibility.

We have investigated the effect of randomly distributed impurities on the transport properties of **unconventional density waves** (UDW) in quasi one dimensional systems. The frequency dependent conductivity of UDW was evaluated for various current directions and gap parameters. The temperature dependence of the threshold electric field of nonlinear conductivity was calculated in an applied magnetic field, and in the presence of imperfect nesting. Comparison with threshold field measurements on the organic conductor α-$(ET)_2$ yielded quantitative agreement, leading us to the conclusion that the low temperature phase of this salt is a UDW. This is further corroborated by our successful interpretation of the observed angular dependent magnetoresistance based on our model. We have also suggested a new mechanism related to UDW, in order to explain the observed "micromagnetism" in the heavy fermion compound URu_2Si_2, and in high temperature superconductors.

The electron dynamics in the normal state of BiSCO is studied by inelastic light scattering over a wide range of doping. A strong anisotropy of the electron relaxation is found which cannot be explained by single-particle properties alone. The results strongly indicate the presence of an unconventional quantum-critical metal-insulator transition where "hot" (antinodal) quasiparticles become insulating while "cold" (nodal) quasiparticles remain metallic. A phenomenology is developed which allows a quantitative understanding of the Raman results and provides a scenario which links single- and many-particle properties.

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Levente Vitos	lv@szfki.hu

Grants and international cooperations

AKP 2000-123 2,2 Quantum disorder and quantum critical behaviour in transition metal compounds (P. Fazekas, 2001-2002)

OTKA T035043 Calculation of electronic states in metal- and oxide surfaces and nanostructures, (J. Kollár 2001-2004)

ESF Network program: Electronic structure calculations (J. Kollár, 1998-2002)

RTN Program: Computational Magnetoelectronics (J. Kollár, 2000-2003)

TÉT D-5/01 Transport properties of highly correlated layered materials (I. Tüttő, 2002-2004)

OTKA T038162 Spin and orbital correlations in solids (P. Fazekas, 2002-2004)

Publications

Articles

C.1. Magyari-Köpe* B, Vitos L, Johansson* B, Kollár J; High pressure structure of $ScAlO_3$ perovskite; *Journal of Geophysical Research*; **107**, NO. B7, 10.1029/2001JB000686, (2002)

C.2. Landa* A, Chang* C-C,. Kumta* PN, Vitos L, Abrikosov* IA; Phase stability of $Li(Mn_{100-x}Co_x)O_2$ oxides: an *ab initio* study; *Solid State Ionics*; **149**, 209-215, (2002)

C.3. Vitos L, Korzhavyi* PA, Johansson* B; Elastic property maps of austenitic stainless steels; *Phys. Rev. Lett.;* **88**, 015501/1-4, (2002); Cover Picture from paper for *Phys. Rev. Lett*. **88**, April 15, (2002)

C.4. Magyari-Köpe* B, Vitos L, Johansson* B, Kollár J; Model structure of perovskites: cubic-orthorhombic phase transition; *Comp. Mat. Sci*.; **25**, 615-621, (2002)

C.5. Magyari-Köpe* B, Vitos L, Grimvall* G, Johansson* B, Kollár J; Low-temperature crystal structure of $CaSiO_3$ perovskite; *Phys. Rev. B*; **65**, 193107/1-4, (2002)

C.6. Magyari-Köpe* B, Grimvall* G, Vitos L; Elastic anomalies in Ag-Zn alloys; *Phys. Rev. B*; **66**, 064210/1-7, (2002);

C.7. Magyari-Köpe* B, Grimvall* G, Vitos L; Erratum: Elastic anomalies in Ag-Zn alloys; *Phys. Rev. B*; **66**, 179902/1, (2002)

C.8. Magyari-Köpe* B, Vitos L, Johansson* B, Kollár J; The origin of octahedral tilting in orthorhombic perovskites; *Phys. Rev. B*; **66**, 092103/1-4, (2002)

C.9. Vitos L, Korzhavyi* PA, Johansson* B; Modeling of alloy steels; *Materials Today*; October, 14-23, (2002)

C.10. Eisenbach* M, Gyorffy* BL, Stocks* G M, Újfalussy B; Magnetic anisotropy of monoatomic iron chains embedded in copper; *Phys. Rev. B*; **65**, 144424/1-7, (2002)

C.11. Brown* G, Lee* HK, Schulthess* TC, Újfalussy B, Stocks* GM, Butler* WH, Landau* DP, Pierce* JP, Shen* J, Kirschner* J; Model of Fe nanostripes on Cu(111); *J. Appl. Phys*.; **91**, 7056, (2002)

C.12. Eisenbach* M, Stocks* GM, Újfalussy B, Gyorffy* BL; Magnetic anisotropy of iron chains embedded in copper; *J. Appl. Phys*.; **91**, 6878, (2002)

C.13. Stocks* GM, Újfalussy B, Shelton* WA, Schulthess* TC, Butler* WH, Canning* A; On the magnetic structure of gamma-FeMn alloys; *J. Appl. Phys*.; **91**, 7355, (2002)

C.14. Fazekas P, Penc K, Berger* H, Forró* L, Csonka* Sz, Kézsmárki* I, Mihály* G; $BaVS_3$: from spin gap insulator to non-Fermi liquid; *Physica B*, **312**, 694-695, (2002)

C.15. Dóra* B, Virosztek A, Maki* K; Magnetic field dependence of the threshold electric field in unconventional charge density waves; *Phys. Rev. B*; **65,** 155119/1-8, (2002)

C.16. Virosztek A., Maki* K, Dóra* B; Micromagnetism in URu_2Si_2 and high temperature superconductors; *Int. J. Mod. Phys. B*; **16**, 1667-1671, (2002)

C.17. Dóra* B, Virosztek A, Maki* K; Imperfect nesting in unconventional density waves; *Physica B*; **312-313**, 571-573, (2002)

C.18. Dóra* B, Virosztek A, Maki* K; Impurity scattering in unconventional density waves; *Phys. Rev. B*; **66**, 1151121/1-10, (2002)

C.19. Venturini* F, Opel* M, Devereaux* TP, Freericks* JK, Tüttő I, Revaz* B, Walker* E, Berger* H, Forró* L, Hackl* R; Observation of an unconventional metal-insulator transition in overdoped CuO_2 compounds; *Phys. Rev. Letters*; **89**, 108003/1-4, (2002)

C.20. Olsson* P, Abrikosov* IA, Vitos L, Wallenius* J; *Ab initio* formation energies of Fe-Cr alloys; *J. of Nuclear Materials*; accepted for publication

C.21. Johansson* B, Vitos L, Korzhavyi* PA; Chemical composition-elastic property maps of austenitic stainless steels; *Solid State Sciences*; accepted for publication

C.22. Dóra* B, Maki* K, Virosztek A; Imperfect nesting and transport properties in unconventional density waves; *Phys. Rev. B*; accepted for publication; (cond-mat/0209288)

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C.26. Vitos L, Abrikosov* I A, Johansson* B; Coherent potential approximation within the exact muffin-tin orbitals theory; In: *Proceedings of IAC-3 conference*; accepted for publication

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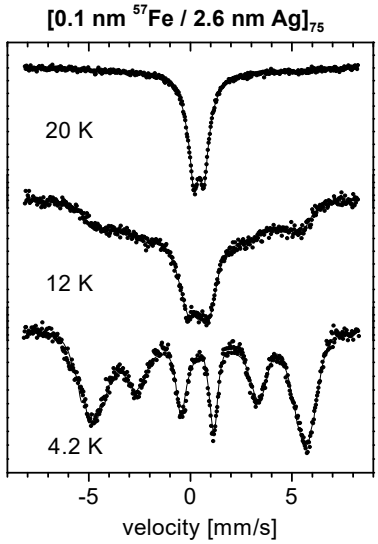
See also H.1.

D. NON-EQUILIBRIUM ALLOYS

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

Superparamagnetic behaviour of nanocrystalline alloys. — One of the most intensively studied topics of solid state physics and material science is the magnetism of nanoscale systems. Superparamagnetism which is characteristic for nanosized magnetic particles is quite important in this respect. Nanocrystalline samples, produced by the controlled crystallisation of amorphous ribbons, are especially useful since fully compact probes are produced with easy control of particle size and packing fraction. The superparamagnetic behaviour of nanocrystalline $Fe_{80}B_{12}Zr_7Cu$ alloys having a different amount of bcc fraction controlled by DSC heat treatments, were studied by high temperature SQUID magnetometry and Mössbauer spectroscopy. The granule diameter calculated from magnetic measurements is significantly higher than the X-ray determined grain size but is proportional to that value. Mössbauer spectroscopy detects the superparamagnetic behaviour at substantially lower temperatures than the macroscopic magnetisation studies. It means that the applied magnetic field significantly influences the superparamagnetic state.

Granular magnetoresistance of Fe/Ag multilayers. — Fe/Ag granular alloys were prepared by sequential deposition with vacuum evaporation of the elements. By decreasing the nominal thickness of the magnetic layers of a multilayer sample causes a gradual transition to a granular system with characteristic superparamagnetic behaviour. The average grain size of the magnetic particles was estimated from the superparamagnetic blocking temperature as measured by Mössbauer spectroscopy and SQUID magnetometry. Mössbauer spectra of a sample with an estimated 1 nm average Fe grain size are shown in the figure which illustrates the rather low blocking temperature. It was shown that with this sample preparation method the average grain size can be varied on the nanometer scale at different compositions. Our samples show giant magnetoresistance behaviour similar to that observed in granular alloys prepared with co-deposition methods. The large resistance change observed up to 12 T applied magnetic field is attributed to spin dependent electron scattering on superparamagnetic grains embedded in a nonmagnetic matrix. Our results indicate that the optimum concentration of the magnetic atoms to observe large magnetoresistance is not universal, but depends on the average magnetic grain size and the temperature.



Mössbauer spectra of a Fe_5Ag_{95} granular alloy measured at the indicated temperatures. The nominal layer sequence is given in the figure.

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Grants and international cooperations

OTKA T 030753 Magnetic systems with nanoscale inhomogeneities (I. Vincze, 1999-2002)

OTKA : T031854 The influence of atomic volume and local environment to the anomalous magnetic properties of equiatomic alloys (T. Kemény, 2000-2003)

OTKA T034602 Magnetic properties of multilayers (J Balogh, 2001-2004)

OTKA T038383 Interaction of superparamagnetic clusters (LF Kiss, 2002-2005)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP9: Nation-wide cooperation for the study of non-equilibrium metallic materials. (T. Kemény, 2000-2003)

Long term visitors:

— Dr. V. Franco, (University of Seville, Department of Physics, Condensed Matter Spain, June, 2002, Host: L.F. Kiss)

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D.3. Balogh J, Vincze I, Kaptás D, Kemény T, Pusztai T, Kiss LF, Szilágyi* E, Zolnai* Z*, Kézsmárki* I, Halbritter* A, Mihály* G; Interface Magnetoresistance of Fe/Ag Multilayers; *Phys. Stat. Sol. (a)*; **189**, 621-624 (2002)

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D.6. Franco* V, Kiss LF, Kemény T, Vincze I; Conde* CF, Conde* A; High temperature evolution of coercivity in nanocrystalline alloys; *Physical Review B*; accepted for publication

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See also F.1., H.3.

E. X-RAY DIFFRACTION

G. Faigel, F. Borondics[#], G. Bortel, L. Gránásy, Z. Jurek, K. Kamarás, G. Klupp[#], É. Kováts[#], G. Oszlányi, S. Pekker, T. Pusztai, M. Tegze

Fullerenes and their compounds. — The fullerenes are closed shell molecules containing only carbon atoms. The most abundant among them is the C_{60} molecule. Even in the simplest form (ie. solids of pure C_{60}) C_{60} is not fully understood. Illumination of the fcc pristine C_{60} by intensive light results in a phototransformation. This was the first case when intermolecular linkage of the fullerene molecules was proposed. We developed a novel method for the production of C_{60}-photopolymer in gram quantities. This method is based on the liquid phase transport of the monomer. The larger quantity of phototransformed C_{60} allowed the separation of the C_{120} cycloadduct dimer in pure form. X-ray powder diffraction revealed a face centered cubic structure with a=14.05 Å lattice constant, which can be well understood starting from the C_{60}-C_{60} intermolecular distance and a disorder of the dimer molecules in the lattice. Further, we isolated higher oligomers with the HPLC technique. Among them there are three different trimers, and several tetramers. The precise determination of the conformation of these oligomers is in progress

X-ray holography with atomic resolution. — In holography, the scattered radiation is mixed with a reference wave and the resulting interference pattern is recorded. The hologram contains both the intensity and the phase information and the 3 dimensional image of the object can be reconstructed. In the last few years we developed hard x-ray holography using inside reference points for the study of the atomic order in solids. However, this method also has limitations, it can image the environment of heavy atoms only. To overcome this, we introduced a new technique, the "angular integrated elastic scattering". Beside the theoretical description, we illustrated the feasibility of this method by x-ray and neutron scattering experiments. For the demonstration experiments we chose a simple compound, the LiF.

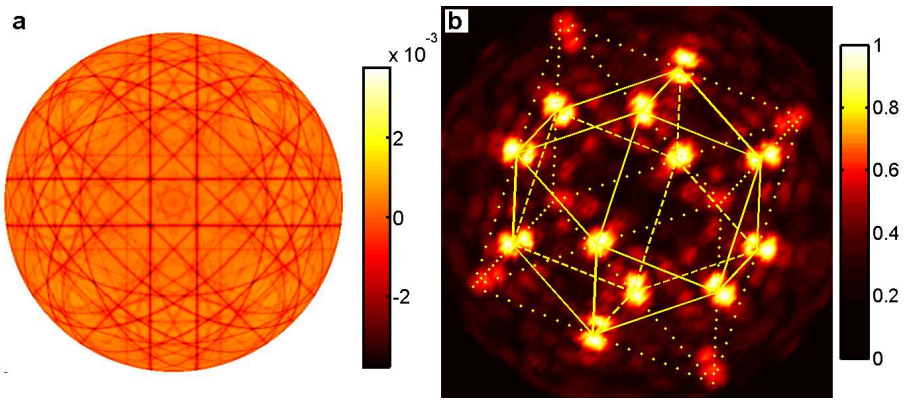

Fig.1. The atomic environment of the F atoms in a LiF crystal, (hologram left panel, reconstructed image right panel).

None of the element of this compound could be used in an x-ray holographic experiment as central atom. Using angular integrated elastic scattering we could image the F atoms.

Theory of phase transformations. — Extending the work done in previous years, we applied field theoretic models to study crystallization in undercooled/supersaturated liquids. We applied the single-order-parameter Cahn-Hilliard theory to deduce properties of the

[#] Ph.D. student

fluid-crystal interface from nucleation experiments on five stoichiometric oxide glasses. The reduced interfacial free energy and the interface thickness, we obtained, cover the $\alpha = 0.28 - 0.51$ and the $d = 0.8 - 1.6$ nm ranges, respectively. For oxide glasses we find that α scales with $n^{-1/3}$, where n is the number of molecules per formula unit.

We developed a phase field theory for polycrystalline solidification, and performed large-scale simulations (10000x10000 grid) to determine the Kolmogorov-exponents for primary dendritic solidification and "soft-impingement" of particles via diffusion fields. Our results are consistent with experimental results. We demonstrated that our model is able to describe other complex solidification morphologies, such as polycrystalline spherulites seen in polymer films or fractal-like polycrystalline patterns forming in electrodeposition. To model the formation of irregular dendritic morphologies seen recently in clay-polymer films, we introduce randomly distributed "orientation pinning centers" into the simulation which are represented by regions of externally imposed orientation. During their engulfment into the crystal, these particles induce the formation of new grains, a phenomenon driven by the impetus to reduce the crystallographic misfit along the particle perimeter by creating grain boundaries within the growing dendritic crystal. We obtained a striking similarity between experiment and simulation (figure 2). The disorder in dendrite morphology originates from a polycrystalline structure that develops during a sequential deflection of dendrite tips on orientation pinning centers.

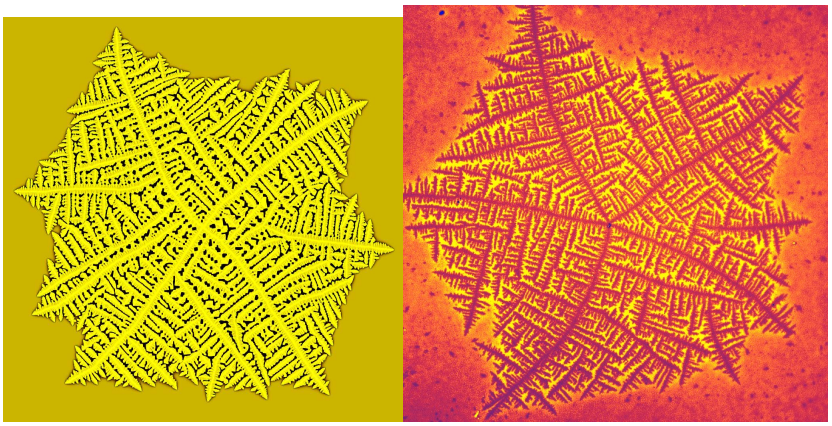

Figure 2. Interaction between foreign particles and denritic growth. On the left: Composition map from phase field simulation. On the right: Experiment on thin polymer blend-clay film (by the courtesy of V. Ferreiro and J. F. Douglas).

We proposed a density functional theory to describe fcc and bcc nucleation in non-equilibrium liquids. We have shown that the increase of the interface free energy with deviation from equilibrium seen in recent Monte Carlo simulations can be recovered if the molecular scale diffuseness of the crystal–liquid interface is considered. The nucleation barrier predicted by our model for small deviations from equilibrium is in a far better agreement with the simulations than the classical droplet model. Remarkably, a minimum of the nucleation barrier, similar to the one seen in polydisperse systems, occurs at high densities if the density dependence of the Ginzburg-Landau coefficients is considered.

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Grants and international cooperations

OTKA T022041 Atomic resolution X-ray holography (M. Tegze, 2001-2004)

ESA Prodex 14613/00/NL/SFe(IC), Modelling of Nucleation and Phase Selection (L. Gránásy, 2000-2003).

OTKA T029931 Structural studies of polymer fullerides (G. Faigel 1999-2002)

OTKA T034198 Temperature and pressure dependent studies of the optical properties of fullerene salts (K. Kamarás, 2001-2004)

OTKA T037323 Dynamics of non-equilibrium morphologies (L. Gránásy, 2002-2005).

Participation in EU IST program FRENDTECH-EAST (IST-2000-30129) (K. Kamarás 2002-2004)

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E.2. Pekker S, Kováts É, Kamarás K, Pusztai T, Oszlányi G; Diffusionless solid state reactions in C_{60} and its supramolecular derivatives: Photopolymerization and host-guest cycloaddition; *Synth. Metals*; **1-3**, 9502, (2002)

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E21. Kamarás K, Nikolou* M, Chen* Z, Rinzler* AG, Tanner* DB; Infrared transmittance of free-standing single-wall carbon nanotube films; In: *International Conference on the Low Energy Electrodynamics in Solids (Montauk, NY, USA, October 13-18, 2002)*; Ed: L. Mihály, http://solidstate.physics.sunysb.edu/lees2002

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See also D.3., D.8.

F. ELECTRON CRYSTALS

G. Kriza, P. Matus[#], L. Németh[#], Á. Pallinger[#], I. Pethes[#], B. Sas

Dissipation in high-critical-temperature superconductors. — In type II superconductors, the dissipation in response to slowly varying electromagnetic fields is dominated by the dynamics of Abrikosov vortices. Material details of the superconductor enter mainly via the "friction coefficient" that gives the vortex velocity in terms of the driving Magnus force. The friction coefficient, in turn, is controlled by the density and relaxation properties of the low-lying "core states", i.e., quasiparticle states localized to the vortex core. It has been found recently, that in layered copper-oxide superconductors, the density of low-energy core states is suppressed by the formation of a concurrent charge or spin order at the vortex cores. To clarify the consequences of these exciting new findings on vortex dynamics, we have performed a systematic investigation of the flux-flow resistance (resistance arising from vortex motion) in high-T_c BSCCO superconductors. We have found that the flux flow resistance is about two orders of magnitude higher than predicted by Bardeen-Stephen law describing "classical" superconductors. We interpret this result in terms of a reduced friction coefficient in agreement with a low density of core states. We have also considered the effects of a vortex flow pattern different from Abrikosov vortices and effects of a reduced core energy.

NMR relaxation in charge-density-wave systems. — On the basis of extensive NMR measurements on a single crystal of $Rb_{0.3}MoO_3$ (blue bronze), we report several aspects of its charge density wave (CDW) and metallic phases that require a reinterpretation of some earlier results and indicate several aspects of the CDW fluctuations that will require further development of the theoretical models to describe them. From measurements of the spin-lattice relaxation rate ($1/T_1$) of both ^{85}Rb and ^{87}Rb, it is clear that the dominant coupling responsible for $1/T_1$ is quadrupolar both above and below the CDW transition. This result contradicts the earlier interpretation that it was magnetic coupling to the conduction electrons above the transition. Also, there is no clear evidence of a coherence peak in $1/T_1$ below the transition. For most orientations of the external field relative to the crystalline axes, $1/T_1$ in the CDW phase is nearly constant across the spectrum of the central NMR transition, in contradiction to the prediction of the simple phason model for the fluctuations. Thus, there are additional fluctuation modes of the CDW that need to be included into the model for $1/T_1$.

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Grants and international cooperations

OTKA T037976 Dissipation in type-II superconductors (G. Kriza, 2002-2004)

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OTKA TS040878 Collective electronic states in solids (G. Kriza, 2002-2004)

Publications

Articles

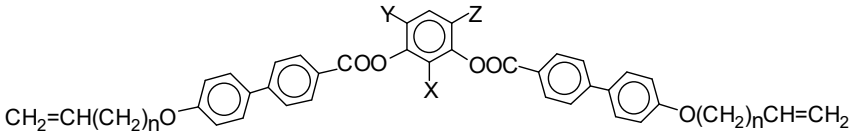
F.1. Portier* F, Kriza G, Sas B, Kiss LF, Pethes I, Vad* K, Keszei* B, and Williams*FIB; Slow relaxation of low-temperature vortex phases in $Bi_2Sr_2CaCu_2O_8$; *Phys Rev B;* **66**, 140511/1-4, (2002); re-published in: *Virtual Journal of Applications of Superconductivity*, **3**(9), 2002 (http://www.vjsuper.org)

F.2. Clark* WG, Tanaka* KB, Vonlanthen* P, Kriza G; New insights on charge density wave and other fluctuations in blue bronze from NMR measurements; *Synthetic Metals;* accepted for publication

G. LIQUID CRYSTALS

Á. Buka, L. Bata, T. Börzsönyi, N. Éber, K. Fodor-Csorba, A. Jákli, I. Jánossy, Sz. Németh[#], T. Tóth-Katona, A. Vajda

A new series of **bent core mesogens** derived from either resorcinol, 2-methyl-, 2-nitro-4-chloro or 4,6-dichloro resorcinol were synthesized giving the substituted 1,3-phenylene-bis 4-(alkenyloxybiphenyl) carboxylates. The chloro-derivatives showed the so called 'banana' nematic phase. The nitro group connected to the central aromatic ring stimulated the appearance of a B7 phase between 50°C and 100°C. This compound is the first one exhibiting the B7 phase at this low temperature range.



New **deuteration** method was developed for the synthesis of 1,3-phenylene-bis 4-[(10-undecenyloxy)benzoyloxy]benzoate-d_4 and 4-chloro-1,3-phenylene-bis 4-[(9-decenyl-oxy)benzoyloxy]benzoate-d_3. These compounds showed unusual behaviour according to ^{2}H NMR investigations.

On some **bent-shape molecules** unique Isotropic-*SmC_G*-*SmCP* phase sequences were observed. The *SmCP* phase has monoclinic chiral C_2, while the *SmC_G* phase has a general chiral triclinic C_1 symmetry, i.e. the lowest symmetry phase occurs directly below the isotropic liquid phase. The observed phase sequences were explained by a phenomenological model.

Free-standing fibers were prepared and studied in liquid crystals of bent-shape molecules. Typical fibers are shown in Figure 1.

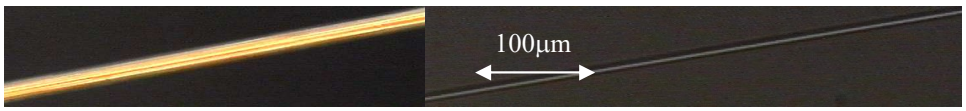


Figure 1: Freely suspended fibers viewed between crossed polarizers. Left side: a bundle of fibers. The length of the entire fiber is 2 mm. Right side: a single fiber. The length of the whole fiber is 1 cm.

In binary mixtures containing a non-polar solvent n-hexadecane dissolved in a bent-core liquid crystal a nanophase segregation of the hexadecane was observed. The phase segregation is due to flexible and steric asymmetries between the flexible solute molecules and the rigid bent cores of the liquid crystal molecules.

The rheological and **piezoelectric response** of a liquid crystalline material was explored around the transition from the ferroelectric mesophase to the solid glassy state.

In homeotropically aligned nematics with negative dielectric anisotropy the **electrohydrodynamic instability** occurs above a bend Fréedericksz transition. In the presence of a magnetic field **H** parallel to the liquid crystal slab, ordered roll patterns with a well defined uniform wavevector $\mathbf{k_{id}}$ appear above the onset of convection. By rotating the cell around an axis perpendicular to the slab by a small angle α, one can manipulate the

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system into a state with wavevector $\mathbf{k} = \mathbf{k_{id}} + \Delta\mathbf{k}$ where $\Delta\mathbf{k}$ is roughly perpendicular to $\mathbf{k_{id}}$. We found that the system restores $\mathbf{k_{id}}$ via defects moving essentially perpendicular to the rolls. The direction as well as the magnitude of the velocity as a function of $\mathbf{k}$ agrees with predictions of the weakly nonlinear theory. In particular, the nonanalyticity for $\mathbf{k}\rightarrow 0$ was proved.

The characteristics of the electroconvection patterns in a homeotropic nematic liquid crystal under the influence of a variable magnetic field were analysed in detail. "Re-entrant" normal rolls (Fig. 2.) were first observed unambiguously at low frequency and a non-monotonic magnetic field dependence of the threshold voltages was detected. We proved that the effect of the magnetic field on the normal roll - abnormal roll transition agrees well with theoretical predictions of the weakly nonlinear analysis.

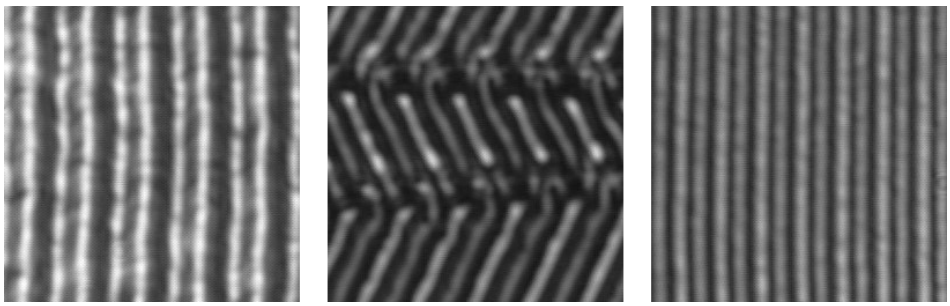

Figure 2. Snapshots of the electroconvection patterns in a homeotropic nematic Phase 5A. "Re-entrant" normal rolls at $f<f_{L2}$ (left), oblique rolls at $f_{L2} < f < f_L$,(middle), normal rolls at $f>f_L$.(right).

Surface effects (interactions with the container walls) influence the **nucleation and growth of smectic B** phase from the nematic in thin samples either in free growth or in directional solidification of a mesogenic molecule (CCH4). In samples coated with rubbed polyimid the orientation effect of SmB crystals is mediated by the nematic, whereas, in monooriented poly(tetrafluoroethylene) coated samples it results from a homoepitaxy phenomenon occurring for two degenerate orientations. The first (diffusional) instability of the propagating front immediately above the Mullins-Sekerka instability threshold was also analysed. The nature of the observed drifting shallow cells was explained by means of a linear stability analysis including diffusive and kinetic anisotropies, and by a numerical approach based on the phase field model with sharp capillary and kinetic anisotropies.

The **interaction of polarized light** with dye-doped high-viscosity fluids was tested in mixtures of glycerin and azo dyes. We showed that at sufficiently low temperatures, significant dichroism and birefringence can be induced at relatively weak continuous wave light intensities (~10mW/cm^2). It was demonstrated that while the dichroism originates fully from the dye, a large part of the birefringence can be attributed to the orientation of the host molecules. The results yielded valuable information about the guest-host interaction in the solutions studied.

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Grants and international cooperations

OTKA T-030401 Synthesis of aromatic and heteroaromatic liquid crystals and study of their physico-chemical properties. (Katalin Fodor-Csorba, 1999-2002)

OTKA T-031808 Convective and interfacial instabilities in liquid crystals. (Ágnes Buka, 2000-2003)

OTKA T-032667 Synthesis of low molar mass, monomeric and polymeric liquid crystals labeled by a stable isotope, and their spectroscopic studies. (Katalin Fodor-Csorba, 2000-2003)

OTKA T-037275 Interaction of liquid crystals and polymer films. (Jánossy István, 2002-2005)

OTKA T-037336 Flow phenomena in liquid crystals. (Nándor Éber, 2002-2005)

MTA-OTKA-NSF Investigation of liquid crystalline mesophases of bent core molecules. (Ágnes Buka, 2002-2005)

MTA-INSA (Hungarian-Indian bilateral) Experimental and theoretical studies on liquid crystals. (Nándor Éber, 2001-2003)

MTA-CAS (Hungarian-Chinese bilateral) Physical and chemical study of liquid crystals. (Nándor Éber, 2001-2003)

MTA-SASA (Hungarian-Serbian bilateral) Structure and physical study of liquid crystals. (Nándor Éber, 2001-2003)

MTA-WATWAW (Hungarian-Polish bilateral) Study of liquid crystals.(Katalin Fodor-Csorba, 2001-2003)

MTA-ASCR (Hungarian-Czech bilateral) Synthesis and study of ferroelectric liquid crystals leading to preparation of mixtures with defined properties. (Katalin Fodor-Csorba, 2001-2003)

MTA-CNR (Hungarian-Italian bilateral) New banana-shaped monomers and their polymer derivatives. (Katalin Fodor-Csorba, 2001-2003)

IC15-CT98-0806 Inco Copernicus Photonic devices: new liquid crystalline composite materials. (István Jánossy, 1999-2002)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP11: Interaction of light with condensed matter. (N. Éber, 2000-2003)

EU-HPCF-CT-2002-00247 Nonequilibrium in physics and in biology.(Ágnes Buka, 2002-2005)

EU-HPRN-CT-2002-00312 Nonequilibrium physics from complex fluids to biological systems. (Ágnes Buka, 2002-2006)

PST.CNS 975474 NATO linkage grant Patterns and chaos in electroconvection of liquid crystals. (Ágnes Buka, 2000-)

NATO-ASI Pattern formation, granular physics and soft condensed matter. (Ágnes Buka, 2002-2003)

COST D14 WG 0015 Advanced molecules and macromolecules containing banana-shaped mesogens for photonic materials. (Katalin Fodor-Csorba, 2002-2004)

Long term visitors

— *Erik Benkler*: Darmstadt University of Technology, Darmstadt, Germany, 1-31 August, 2002 (KFKI-CMRC grant, host: I. Jánossy).

— *David Statman*: Alleghiny College, Meadville, Pennsylvania, USA, 1 January - 31 August, 2002 (Fullbright scholarship, host: I. Jánossy).

— *Wojciech Otowski*: Cracow University of Technology, Cracow, Poland, 1 January - 8 Mai, 2002 (KFKI-CMRC grant, host: Á. Buka).

— *C.V.Yelamaggad*: Centre for Liquid Crystal Research, Bangalore, India, 13 July - 11 August, 2002 (INSA-HAS exchange program).

— *Stanislaw Rozanski*: Higher Vocational State School in Pila, Pila, Poland, 1 July – 31 December, 2002 (KFKI-CMRC grant, host: N.Éber).

— *Elzbieta Kochowska*: Cracow University of Technology, Cracow, Poland, 1 November – 31 December, 2002 (EU-RTN grant, host: Á.Buka).

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Articles

G.1. Catalano* D, Cifelli* M, Domenici* V, Fodor-Csorba K, Richardson* R, Veracini* CA; ^{2}H NMR and SAXS of a ferroelectric liquid crystal: Unwinding of the ferroelectric chiral helix by high magnetic fileds; *Chem Phys Lett;* **346**, 259-266, (2001).

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G.18. Jákli A; Scattering displays from banana-smectics; *Liquid Crystals Today*, **11**, 1-6, (2002).

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G.20. Börzsönyi T, Akamatsu S*, Faivre G*; Surface effects in nucleation and growth of smectic B crystals in thin samples; *Phys Rev E;* **66**, 051709/1-14, (2002).

G.21. Vajda A, Kaspar* M, Hamplova* V, Bubnov* A, Fodor-Csorba K, Éber N; Phase diagrams and physical properties of binary ferroelectric mixtures based on a series of chiral α-cyanocinnamate derivatives; *Liquid Crystals*; **29**, 1347-1354, (2002).

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G.23. Stojadinovic* S, Adorjan* A, Sprunt* S, Sawade* H, Jákli A; Dynamics of the nematic phase of a bent core liquid crystal; *Phys Rev E*; accepted for publication.

G.24. Mátyus* E, Fodor-Csorba K; Synthesis and liquid crystal properties of new banana-shaped cinnamoyl derivatives; *Liquid Crystals;* accepted for publication.

G.25. Jákli A, Nair* GG, Sawade* H, Heppke* G; A bent-shape liquid crystal compound with antiferroelectric triclinic-monoclinic phase transistion; *Liquid Crystals*; accepted for publication.

G.26. Vajda A, Hamplova * V, Kaspar* M, Bubnov* A, Obadovic* DZ, Éber N, Fodor-Csorba K; Structure-property relationship studies on chiral lactic acid derivatives; *J of Research in Physics*; accepted for publication.

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See also E.5., E.7., E.19.

H. METAL PHYSICS

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

Metal-hydrogen systems. — In the ^{1}H NMR study of **Zr_yNi_{1-y}-H** amorphous alloy-hydrogen systems, from the NMR characteristics the parameters describing the mobile and residual hydrogen were selected and the quantity of both components were measured. The magnitudes of the residual component are in good correlation with the probabilities of 4Zr tetrahedra in these alloys. This result influences the interpretation of the spin lattice relaxation time (T_1). The evaluation of T_1 and the shift terms (Knight and chemical shifts) are in progress, and the expected conclusions will reflect the hydrogen motion and the electronic structure of the system.

High purity **Pd** and **Pd_{1-x}-Ag_x** (x=0.1, 0.2 and 0.35) alloys were charged with hydrogen, and the NMR free induction decay (FID), different echoes, T_1 and $T_{1\rho}$ spin-lattice relaxation time in the laboratory and rotating reference systems, respectively, were measured down to 2.4 K on this fcc crystalline alloy, on a model material representing a chemically disordered system for hydrogen storage materials. Samples of H/M=0.04….0.7 hydrogen content were prepared and investigated. In the very low temperature range (2-3 K), inhomogeneous echoes were detected near the commonly known solid echoes suggesting a strong paramagnetic contribution to the proton NMR spectrum of unknown origin. The substantial dipole-dipole contribution to the spectrum and to the echoes in the smallest hydrogen content reveals hydrogen clustering that contradicts the statement of the generally accepted lattice gas model for the α phase.

Looking for new fields of NMR research.

— **NMR on nanocrystalline copper. —** Quadrupole effects in the room temperature continuous wave ^{63}Cu NMR spectra, the shortening of the "$\pi/2$" pulse length and the echo amplitudes following two-pulse generation were investigated on nanocrystalline copper powders. Systematic measurements on the parent polycrystalline copper and on copper based Cu-Pd dilute alloys based on the same experimental basis were also made. Different NMR responses show different electric field perturbation ranges existing in this heterogeneous material.

— **Cycloadditivity of carbon materials.** — Heterogeneous Diels-Alder reaction between cyclopentadiene and different solid carbons (carbon black, graphite, activated carbon and multi-wall carbon nanotubes) were studied by proton NMR measurements. The analysis of FID and echo signals showed that the applied reactants formed covalent bonds with the carbon materials to different extents. The relative amounts of the bound cyclopentadiene were determined by NMR spectroscopy and thermal analysis.

— **Hydration of semi-structured proteins. —** Temperature dependence of NMR FID signal amplitude of water protons was studied in the physiological solutions of two semi-structured proteins, namely hCSD1 and MAP2C and as a reference material of structured protein BSA, moreover in the buffer solutions. A step observed at about –6 °C…-12 °C shows that the mobile ("free") fraction of water freezes and an immediate decrease is indicated in the FID amplitude. The differences in the magnitude and the temperature dependence of FID amplitudes below the mentioned transition range reveal the different nature and quantity of non-freezible ("bound", that is the hydrate layer of) water in the investigated samples. There is a substantial difference in the quantity of bound water in the water solutions of semi and totally structured protein.

GMR in metallic multilayers. — It has been demonstrated that Co(Ru)/Ru multilayers with a hexagonal close-packed structure can be produced by electrodeposition. For appropriate layer thicknesses, a clear giant magnetoresistance (GMR) behaviour has been found. The observed GMR is very small (less than 0.1 % for 8 kOe at room temperature) but not smaller than the GMR of Co/Ru multilayers prepared previously by high-vacuum methods. It is argued that neither structural imperfectness of the multilayers nor chemical intermixing at the interfaces can be the main reason for the small GMR observed in the Co-Ru system for any preparation technique. It is suggested that the strongly reduced spin-dependent scattering characteristics of the interfacial Co-Ru alloys might explain the low GMR of Co/Ru multilayers. Namely, it turned out from room-temperature electrical resistivity and magnetoresistance studies of electrodeposited Co metal and Co(Ru) dilute alloys that the incorporation of a small amount of Ru into Co significantly reduces the anisotropic magnetoresistance (AMR). The influence of Ru on the AMR of Co is explained by a drastic change of the asymmetry of d-band spin-up and spin-down electronic states at the Fermi level as revealed also by recent electronic band-structure calculations on Co-rich Co-Ru alloys.

In another study, the room-temperature magnetoresistance (MR) and magnetization characteristics were investigated for electrodeposited Ni-Co-Cu(3nm)/Cu(d_{Cu}) multilayers with d_{Cu} = 1 nm and 2 nm as a function of the ratio of Co to Ni in the magnetic layer. The maximum GMR was obtained when the Co and Ni contents of the magnetic layer were approximately equal for d_{Cu} = 1 nm, whereas a significantly smaller GMR with no systematic dependence on Co-content was observed for d_{Cu} = 2 nm. Concurrent increase of the coercive field (H_c) and the MR peak position (H_p) with Co-content was observed for d_{Cu} = 1 nm up to a Co:Ni ratio of 1:1, beyond which H_p increased faster than H_c, with $H_p \approx 2H_c$ when the ratio reached ~ 4:1. For films containing approximately equal quantities of Co and Ni, the MR vs H curves could be successfully fitted by a Langevin function. This was interpreted by ascribing the magnetization contribution for magnetic fields above about $2H_c$ to superparamagnetic (SPM) regions which form due to the electrochemical deposition conditions between the non-magnetic Cu layer and the ferromagnetic (FM) Ni-Co-Cu layer. The formation of such intermixed interfaces is a general phenomenon in electrodeposited multilayers, leading to a strongly reduced antiferromagnetic coupling of the magnetizations of the neighbouring FM layers. In such cases, the observed GMR curves exhibit a typical concave shape and arise due to the slowly saturating SPM behaviour at the intermixed interfaces.

Hydrogen permeation and entrapment kinetics in metals. — A simulation program has been developed to analyze hydrogen entrapment during hydrogen permeation experiments where the input side hydrogen concentration is constant and the exit side hydrogen concentration is zero. The simulations performed focused on the effect of traps on the exit side hydrogen flux and that on the capture and release of hydrogen by traps as a function of the distance from the entry surface. The number of dimensionless parameters to be defined in the presence of traps was much higher than in the absence of traps. It was found that in several cases the first breakthrough time of hydrogen is a linear function of the trap concentration. However, when the capture of hydrogen by traps is slow, the permeation curve may have a very unusual shape, and the trap saturation profile changes substantially during the permeation experiment. The impact of the hydrogen entrapment kinetics on the result of permeation experiments in connection with the industrial test of enamel-grade steel plates was also studied.

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Grants

OTKA T 031994	Random walk and diffusion of hydrogen in alloys (K. Tompa, 2000-2002)
OTKA F 032046	Preparation of metallic multilayers from compositionally modulated flowing electrolytes (L. Péter, 2000-2003)
OTKA D-38490	Study of potential hydrogen storage materials (M. Bokor, 2001-2002)
OTKA T 037673	Tunnelling magnetoresistance (TMR) in ferromagnetic/insulator nanostructures (I. Bakonyi, 2002-2005)
OM ALK-00038/01	Raw materials and test methods for the enamel industry (2002-2003, participating scientist: L. Péter)

Long term visitors

— N. Sulitanu, University A.I. Cuza, Iasi, Romania; Jan. 6 – Mar. 6, 2002 (NATO Science Fellowship, host: I. Bakonyi)

— M. Alper, Uludag University, Bursa, Turkey; July 1 – July 31, 2002 (NATO Science Fellowship, host: I. Bakonyi)

— B. Zagyi, Technical University of Kosice, Slovakia; Oct. 9 – Nov. 8, 2002 (Domus Hungarica Fellowship, host: L. Péter)

— L. Novák, Technical University of Kosice, Slovakia; Oct. 9 – Nov. 8, 2002 (Domus Hungarica Fellowship, host: L. Péter)

Publications

Articles

H.1. Bakonyi I, Babic* E, Miljak* M, Lück* R, Bahle* J, Hasegawa* R, Kollár J; Magnetic properties of amorphous, crystalline and liquid Ni-B alloys; *Phys Rev B;* **65**, 104423/1-10; (2002)

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H.8. Cziráki* Á, Péter L, Arnold* B, Thomas* J, Bauer* HD, Wetzig* K, Bakonyi I; Structural evolution during growth of electrodeposited Co-Cu/Cu multilayers with giant magnetoresistance; *Thin Solid Films;* accepted for publication

H.9. Péter L, Almási* B, Verő* B, Schneider* H; Theoretical analysis of entrapment kinetics in hydrogen permeation experiments; *Mater Sci Eng A;* accepted for publication

H.10. Péter L, Almási* B, Verő* B, Schneider* H; Theoretical analysis of hydrogen permeation and entrapment kinetics; *Materials Science Forum;* **414-415**, accepted for publication

H.11. Tompa K, Bánki P, Bokor M, Lasanda G, Vasáros* L; Diffusible and residual hydrogen in amorphous Ni(Cu)-Zr-H alloys; *J All Comp*; accepted for publication

Book

H.12. Szalma* J, Péter L, Szetey* Z*; Fizikai-kémiai gyakorlatok biológus hallgatók számára, egyetemi jegyzet (Laboratory practice in physical chemistry for biology major students, textbook for students, in Hungarian); Eötvös University, Faculty of* Sciences, Budapest, 2000; pp. 1-212.

See also: I.1., I.13., I.15., J.15.

I. METALLURGY AND MAGNETISM

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

Soft magnetic nanocrystalline alloys. — New families of iron based bulk amorphous alloys have been developed based on industrial materials like: cast iron, W8 type "silver" steel, R2 type "rapid" steel, etc., by adding several weight percentages of boron and phosphorus. These elements have been introduced also from industrial Fe-B and Fe-P alloys. In this way, cheap bulk amorphous alloys can be obtained for various practical applications for producing small-size construction elements, such as cogwheels, gears, rack and pinion, bevel wheels, etc. A rule of thumb has been deduced from the statistical processing of literature data in order to help the search for new bulk amorphous alloys: the crystallization temperature must be larger than the half of the melting temperature. A new family of nanocrystalline alloys was developed based on phosphorus instead of boron. We are continuously searching for the optimal composition. At the time being, the best composition is $Fe_{81}P_{13}Si_2Nb_3Cu_1$ which is prepared from cheep industrial Fe-P alloy and can be cast in amorphous ribbon precursor form simply in air. The nucleating element Cu suppresses the first crystallization temperature, increasing in this way the temperature distance between the two stage of crystallization. Nb is the grain growth inhibitor element like in the former nanocrystalline alloys. A new high temperature Co-based nanocrystalline alloy was developed which can be cast in air: $Fe_{85-x}Co_xNb_5B_8P_2$. For x = 20, this material proved to exhibit flat hysteresis loop obtainable by simple annealing at 500 ^oC/1h, without any magnetic field or stress annealing. This phenomenon might be correlated with the shape asymmetry of the Fe-Co nanograins which is reflected also in the Avrami exponent n=1.1. Although the details of this phenomenon is worth for further electron-microscopic investigations, it is of great practical importance since it enables to avoid the costly field and stress annealing. The random walk assumption of the Herzer model was tested directly by micromagnetic simulations. The domain wall width enlarges as $1/d^3$ as expected from scaling arguments of Herzer. Micromagnetic simulations have been used to support the mean field arguments of the dipolar ferromagnetic coupling of nanograins above the Curie temperature of the residual amorphous matrix. By using these fundamental results, new nanocrystalline ribbon cores were developed, tested and applied in switch-mode power supply.

Scanning electron microscopy. — The JSM840 SEM equipment of the laboratory provides the chemical analysis of materials by using an electron probe microanalysis (EPMA) facility. For bulk samples, the analysed sample volume is 1 μm^3 (for thinned samples which can be prepared by the ion-milling gun of the laboratory, this volume is 1/1000 μm^3). In this year, we could replace the old ORTEC analyser of the SEM microscope by a new RÖNTEC EDX Spectrometer EDWIN. This system includes a RÖNTEC UHV Dewar detector with super light element window for the detection of elements from boron (atomic number: 5) upward, the EDWIN Basic System (signal processing unit, data acquisition and display hardware and software) as well as various data evaluation and imaging softwares.

Temperature-modulated thermal and thermomagnetic analysis of amorphous alloys around magnetic and structural phase transitions. — Strong thermal effects are associated with first order phase transitions such as nanocrystallization or formation of a

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new compound. These transitions are irreversible. In contrast, thermal effects associated with a magnetic transformation at the Curie point of an amorphous phase are very weak. The effects appear as small changes in the heat capacity, associated with the loss of the spontaneous magnetization. In the case of small thermal effects, the temperature-modulated differential scanning calorimetry (DSC) increases the instantaneous heating rate and separates the heat capacity change from such apparatus effects like baseline curvature. As a result, the sensitivity for detecting the Curie temperature by DSC is greatly enhanced. In both thermomagnetic (TMAG) and DSC measurements, the application of the temperature modulation technique provides useful results and allows distinguishing between reversible and irreversible processes. The combination of this technique was applied to find a relation between thermal and thermomagnetic effects associated with structural phase transitions of $Fe_{85-x}Cr_xB_{15}$ amorphous alloys ($0 \leq x \leq 11.5$). The measurements were carried out in the range from room temperature up to the Curie point of iron. The phases formed upon heating at high temperatures were identified by X-ray diffraction. A diagram containing the phase transformations obtained from the experimental data could be established for this alloy system.

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Grants and internationa cooperations

OTKA T-034666 Iron-based bulk amorphous alloys and nanocomposites (L.K. Varga, 2001-2004)

OTKA T-035278 Correlation between domain structure, dynamical magnetic properties and structural factors in soft magnetic equilibrium and metastable alloys (2001-2004). The RISSPO is subcontractor (project leader: P. Kamasa) in this research grant of the Budapest University of Technology and Economics.

OTKA T-037643 Nanostructured functional coatings (2002-2005). The RISSPO is subcontractor (project leader: L.K. Varga) in this research grant for the Chemical Research Center of HAS.NATO Science for Peace Project 971930: Magnetic nanocomposites for transformer cores and magnetic refrigeration (L.K. Varga, 1999-2003)

OMFB grant "NATO 00002/99": Matching fund to NATO SfP Project 97/1930 (L.K. Varga, 1999-2002)

EU grant CRD2-2000-30349: Soft magnetic nanomaterials for high temperature and high frequency functional application in power electronic (L.K. Varga, 2001-2004)

NKFP3-00164/2001 Széchenyi NRP: Nanotechnology. (Participating scientist: L. Pogány, 2001-2003).

NKFP-3A/0050/2002 Széchenyi NRP: Development of nanostructured coatings with unique properties by using environmental friendly methods (Participating scientist: L.K. Varga, 2002-2005)

TéT E-9/2001 Preparation of new nanocomposite materials and their applications in materials engineering (L.K. Varga, 2001-2003, Hungarian-Spanish Bilateral Science and Technology Cooperation)

TéT F-36/00 Soft magnetic nanocomposites: preparation, characterization and application in high-frequency power electronics (L.K. Varga, 2001-2002, Hungarian-French Bilateral Science and Technology Cooperation)

HAS-PAS Investigation of thermophysical properties of coatings (P. Kamasa, 2002-2004, Hungarian-Polish Academy Exchange Programme)

Biological Research Center of HAS, Szeged: Contract for constructing a spectrofluorimeter (P. Kamasa, 2002)

Long term visitors

— B. Varga, Transsylvanian University, Brasso, Romania; Jan. 2 – Mar. 31, 2002 (NATO Science Fellowship, host: L.K. Varga)

— A. Concustell, Universitat Autónoma Barcelona, Spain, Sept. 28 – Oct. 27, 2002 (supported by bilateral project TéT E-9/2001, host: L.K. Varga)

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Articles

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I.2. Kamasa P, Myslinski* P; Thermal analysis of the ferromagnetic materials in the region of Curie temperature by temperature-modulated DTA; *Czech J Phys;* **52**, 159-162, (2002)

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I.12. Chakrabarti* PK, Mazaleyrat* F, Varga LK; Soft magnetic properties of rapidly quenched pig-iron-based alloys; *J Magn Magn Mater;* accepted for publication

I.13. Kamasa P, Buzin* A, Pyda* M, Kovac* J, Cziráki* Á, Lovas* A, Bakonyi I; Temperature-modulated thermal and magnetic analysis of amorphous alloys around magnetic and structural phase transitions; *J Magn Magn Mater*; accepted for publication

I.14. Révész* Á, Concustell* A, Varga LK, Surinach* S, Baró* MD; Influence of the wheel speed on the thermal behaviour of $Cu_{60}Zr_{20}Ti_{20}$ alloys; *Mater Sci Eng A*; accepted for publication

I.15. Révész* A, Varga LK, Nagy* PM, Lendvai* J, Bakonyi I; Structure and thermal stability of melt-quenched $Al_{92-x}Ni_8(Ce,Sm)_x$ alloys with x = 1, 2 and 4; *Mater Sci Eng A*; accepted for publication

See also H.4., H.5.

J. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

L. Rosta, L. Almásy#, L. Cser, , I. Füzesy, J. Füzi, A. Len#, E. Rétfalvi#, L. Riecsánszky, Zs. Sánta#, Gy. Török

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 basic and applied research, commercial utilisation and education. 2002 was a very important year for us as we had a complete operating period after the installation of the new cold neutron research facility started in February last year. This ensemble of equipment consists of the liquid hydrogen cold neutron source, the optimised supermirror neutron guide system and a set of experimental stations. Experiments were completed by the local staff and in collaboration with national or foreign users coming from university, industrial or other research laboratories. We operate at BRR a small angle scattering (SANS) instrument, a reflectometer (REFL) and a triple axis spectrometer (TAS). Our activity is based essentially on experiments performed on the above spectrometers, some special studies, however, were performed at other neutron source facilities e.g. at ILL-Grenoble, HMI Berlin or LLB Saclay (France) where we shared the construction of the Spin-Echo spectrometer (MESS).

The scientific activity of our team is focused on three major topics in condensed matter research, namely the investigation of structure and dynamics of *liquids, soft materials* as well as materials properties of *solids.* A considerable effort of our team is also devoted to problems on neutron optics as well as the development of neutron scattering techniques.

Liquids. — Small-angle neutron scattering (SANS) was used to reveal nano-scale structural changes in water-based *ferrofluids* following the external magnetic field turning off. The observed changes in the scattering behavior show a significant aggregation effect stimulated by both the turning on and the turning off of the magnetic field. In some cases the aggregation process takes place long after the magnetic field is turned off. The character of these processes depends crucially on the volume fraction of the magnetic material in the fluid.

Binary *aqueous solutions* of small organic molecules were studied by applying small-angle scattering method together with the thermodynamic theory of Kirkwood and Buff. In the case of methylpyridines two trends in the solution properties have been determined. With increasing number of methyl groups on the pyridine ring, the mixtures exhibit an increasing tendency to form a strongly heterogeneous structure. This means that different regions with strongly different compositions appear in the macroscopically homogeneous solutions. Another trend is the dependence of the non-ideality on the strengths of the solute–water hydrogen bond; the latter can be varied by changing the position of the methyl group on the pyridine ring. A comparison of the structures of 2MP, 3MP and 4MP solutions showed no explicit dependence of the degree of non-ideality with the strength of the solute-water interaction, neither with the appearance of immiscibility regions on the phase diagrams in some of the methylpyridine solutions. These experimental results suggest for instance, that the strength of the hydrogen bond between the two different molecules is not the only, and

Ph.D. student

probably not the most important parameter responsible for the phase separation and for the reentrant phase behavior in aqueous solutions.

Soft materials. — Poly(vinylpyrrolidone) (PVP)-tetraphenylporphyrin (TPP)-C_{60} complexes in heavy water at concentration 1 wt% have been studied at 20 ºC. Starting from *PVP+TPP-complex* and doping it with C_{60} up to C~6 wt%, we revealed the structural evolution from mass fractals with dimension D_M~2.3 at C = 0 wt% to fractals having surface dimension D_S ~2.8 at C~2 wt% and again to mass fractals, $D_M(C)$~2.9-2.8 at C~5-6 wt%. These structural peculiarities can be explained as a result of cross-linking action of the fullerene, forming a microgel substance above the critical concentration C^*~1 wt%. The networking in overdoped complexes (C~5 %wt) is degraded, this indicates a strong influence of the fullerene on water structure.

The *poly(N-vinylcaprolactam)* (PVCL) is a synthetic analogue of several type of biomolecules (enzymes, proteins). It demonstrates a specific hydration and undergoes a coil-globule transition. The PVCL-D_2O system (PVCL mass $M = 1 \cdot 10^6$) has been investigated by SANS at T = 23-43 ºC to reveal the structural features of a collapse at concentration C = 0.5 wt% near the threshold of the coils overlap. (The collapse leads to the segregation of the phase enriched with polymer at T>32ºC). The SANS-experiments at q = 0.1-5 nm^{-1} (scales from a monomer unit to a globule with a gyration radius R_G~16 nm) have shown a stretched coil-globule transformation in the range 32-37 ºC. Using a high-resolution SANS (q = 0.002-0.02 nm^{-1}) we examined the globules' association to a fractal structure (sponge-like) with surface dimension D_F~2.4-2.6. The co-existence of globules and disordered chains (regions of ~5-10 nm) was found. The growth of the content of globular phase was induced by the conformational transition in disordered molecular fragments from coiled (dimension D ~ 1.8) to stretched chains (D~1.2).

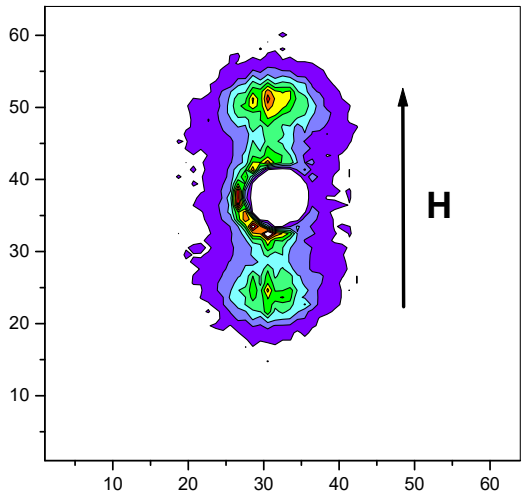

Figure 1. Small angle neutron scattering from the chloroplast thylakoid membranes, when external magnetic field is applied (H=1.2T)

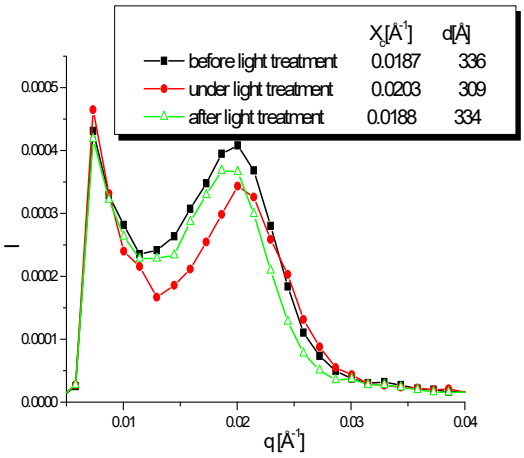

Figure 2. The change of the intensity and position of the SANS diffraction peaks before, under and after light illumination

The photosynthetic machinery in green plants is constituted by a series of proteins and pigments-protein complexes associated with the *thylakoid membranes* of chloroplasts. The thylakoid membrane is continuous through the chloroplast and is folded into stacked region (grana) and un-stacked regions (stroma), respectively. The multilayered grana regions are

characterised by a repeat distance of ∝ 10nm and the system is thus well suited for small angle x-ray (SAXS) and neutron (SANS) scattering studies with the aim of investigation the structural adaptability. We have studied freshly isolated pea and spinach thylakoid membranes suspended in different media and subjected to different light treatments. The functioning of the photosynthetic apparatus was monitored using chlorophyll fluorescence. All systems were aligned in a magnetic field of 1T. SANS spectra from non-oriented samples showed isotropic rings of scattering while the scattering pattern became highly anisotropic when the magnetic field was turned on (Fig.1). Two clear peaks were identified in the q-range 0.005-0.02 nm^{-1} using SAXS, while another peak was seen at 0.002nm^{-1} with SANS (Fig.2). We ascribe the high q features to originate from the grana stacking while the features below 0.003nm^{-1} originate in the semi-periodic arrangement of the stroma lamellae. The intensity and position of the structural features are influenced both by illumination in strong light and by changing the osmotic pressure difference across the membranes by changing the sorbitol concentration of the suspending medium. Thus, in elucidating the nature and mechanism of the adaptation of plants to different environmental conditions, small-angle scattering measurements on fully functional thylakoid membranes carry structural information.

Solids. — The microstuctural evolution of plastically deformed *stainless steel* has been studied. The samples were pulled in the typical bench to cause different plastic deformations. We examined a samples series consisting of several pieces from non-deformed state to broken state. The development of internal surface via intensive growth of pores (voids, size ~20-40 nm) has been observed and a linear decrease of the surface fractal dimension $2.9 \geq D(S) \geq 2.1$ was found by elongation at S=0-60%. The observed scattering features can be used to design the fracture criteria at microscopic level.

Portland cement pastes consist of many crystalline and non-crystalline phases in various ranges of sizes (nm and μm scale). The crystalline phases are embedded in amphorous phases of hydration products. We have investigated the structural changes of hydrating phases in the time interval of 0-30 days. The small angle neutron scattering of Portland cements prepared with a water-to-cement ratio from 0,3 to 0,8 gave us information about the microstructure changes in the material. An important variation of fractal dimension depending on the preparation-to-measurement time interval and water-to-cement ratio was observed.

Archaeological marbles were studied since the method of the small angle neutron scattering is very suitable to investigate the morphology of samples collected from different territories. The SANS patterns indicated characteristic difference between the samples originating from different places, and were very similar when the territory (mine) was the same. An anisotropic pattern seems to be a “signature” of the place, making it possible to identify the provenance of some historical objects. The size and shape distribution of inhomogeneities (micropores), calculated from the scattering patterns can be specific for the geological history of marbles.

Neutron optics. — The experimental realization of the *neutron holographic experiment* is the main achievement in the field of neutron optics in year 2002. We have proposed, that atomic resolution holography can be achieved even by two approaches. The inside source concept uses nuclei possessing of large incoherent scattering cross section. The inside detector concept uses the principle of the optical reciprocity where the positions of the source and the detector are interchanged. Both of these approaches operate with thermal neutrons having wavelength less then the inter-atomic distance in a crystal. In our experiment described below we used the inside detector concept to image lead nuclei in a

$Pb_{0.9974}$ $Cd_{0.0026}$ crystal. Here Cd acts as the internal neutron detector. The number of absorptions depends on the total neutron wave field at the Cd site, including the interference between the directly-arriving and previously-scattered neutrons. After absorbing a neutron, the converted Cd isotope emits gamma radiation while transiting to the ground state, and those gamma rays provide the data for the hologram. Shown here is the reconstructed hologram of the 12 nearest neighbours to a Cd nucleus in the crystal (Fig.3). We not only found the correct lattice parameter (4.93 Å) but also determined the sample's orientation in the neutron beam.

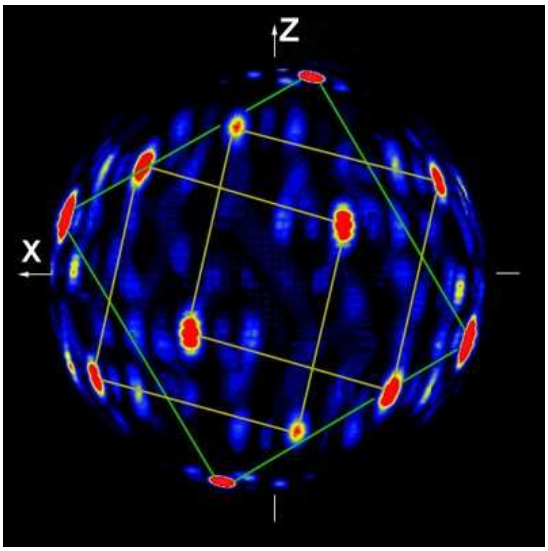

Fig.3. The spots represent the positions of the twelve Pb atoms forming the first neighbours of the Cd nucleus. They are displayed on the surface of a sphere with a radius of 3.49 Å = a/√2, a - being the lattice parameter. The X-axis is the incident beam direction, the Z-axis is the z direction in the system of coordinates of the D9 diffractometer at ILL-Grenoble.

Developments in neutron scattering techniques. — Hybrid adiabatic/non-adiabatic neutron *spin-flippers* (efficiency≥95%) on magnetized thin foils have been designed for a wide wavelength band, $\lambda_{max}/\lambda_{min} \sim 10$. A great interest has been demonstrated for using these compact devices (a few tenth of μm in thickness) as π/2- and π-rotators; various polarized neutron instruments (SANS, reflectometers, NSE, etc.), operating in the range of λ=0.2-2.0 nm, can be constructed for time-of-flight type of instruments.

Magnetic neutron lenses have been designed and constructed using brick-shaped NdFeB permanent magnets and their neutron beam focusing properties tested by numerical simulations and neutron experiments. The magnetic field in the air-gap of a hexapole magnet was computed by means of the integral equation method and measured for the constructed magnets. Hexapole lenses with constant 40000 T/mm^2 and aperture diameter 7 mm have been realised and the neutron beam focusing effect has been demonstrated.

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Grants and international cooperations

EU ERB PL96-9007 Neutron Round Table (L. Rosta, 2001-2004)
ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP1: Enhancing regional users' access to the new Cold Neutron Facility at the Budapest Research Reactor (L. Rosta, 2000-2003)
HPRI-CT-1999-00099 Acces to Research Infrastructure (BNC, L. Rosta, 2000-2003)
HPRI-1999-50016-CT European Polarized Neutron Initiative (Gy. Török 2000-2003)
IAEA B5-HUN/8879 Condensed matter research (L.Cser, 2000-2002)
OMFB 01582/02 Research & development of neutron optical devices (L. Rosta, 2002-2004)
OMFB 01718/02 Development of particle beam chopper system (L. Rosta, 2002-04)
OMFB-00367/02 Magnetic neutron optical devices (L. Rosta, 2002-03)
OM –02617/1999 Large Area Neutron Detectors (L. Rosta, (2000-2002)
OTKA T 22486 Investigation of sintering processes (P. Harmat, E. Rétfalvi, 1999-2002)
TÉT F-25/99 "Balaton" Neutron Detector Systems (L. Rosta 2000-2002)
HAS-RAS 10 Russian Academy: Cold neutron research (L.Rosta, 2002-04)
HAS-RAS 11 Russian Academy: Surface structures (L.Cser, 2002-04)
HAS-RAS 12 Russian Academy: Nanostructures (L.Cser, 2002-04)
HAS-RAS 25 Russian Academy: Water solvent structures by neutron and X-ray scattering (L. Almásy, 2002-04)
HAS-RAS 29 Russian Academy: Structure of biological macromolecular systems by neutron scattering (Gy. Török, 2002-04)
HAS-Dubna JINR Dubna: SANS investigation of liquids (L. Rosta, 2002-03)
HAS-Dubna JINR Dubna: Structure of binary liquids (L. Almásy, 2002-03)

Long term visitors

— V. T. Lebedev, St.Petersburg Nuclear Physics Institute, 1 April-30 June (Host: Gy. Török)

Publications

Articles

J.1. Almásy L, Cser L, Jancsó* G; Kirkwood-Buff integrals in aequous solutions of 3-methylpyridine; *Journal of Molecular Liquids;* **101,** 89-98, (2002)

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J.12. Avdeev* MV, Balasoiu* M, Török Gy, Bica* D, Rosta L, Aksenov* VL, Vekas* L; SANS study of particle concentration influence on ferrofluid nanostructure; *J Mag Mag Mat*; accepted for publication

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J.14. Füzi J; Analytical approximation of Preisach distribution functions; *IEEE Trans Mag*; accepted for publication

J.15. Almásy L, Bánki P, Bellissent-Funel* MC, Bokor M, Cser L, Jancsó* G, Tompa K, Zanotti JM; QENS and NMR studies of 3-picoline-water solutions; *J. Appl. Phys A*; accepted for publication

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J.21. Füzi J, Iványi* A, Török Gy, Rosta L; Optimal design of neutron lens electromagnet; In: *Proc. 8th International Conf. on Optimization of Electric and Electronic Equipment - OPTIM'02, Transilvania Univ. Brasov, 2002*; vol I, pp 17-22, (2002)

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Book Chapter

J.27. Cser L, Salma* I, Molnár* G; Anyagvizsgálatok Neutronokkal (Materials Studies by Neutrons, in Hungarian); *Nukleáris tudomány és a 20. század; Műhelytanulmányok sorozat* (Strategic Research at the Hungarian Academy of Sciences), Eds: Glatz F, Vértes A; MTA, ISSN 1419-1822; pp. 75-90, (2002)

K. NEUTRON SCATTERING

E. Sváb, I. Harsányi[#], Gy. Mészáros, L. Pusztai, Z. Somogyvári[#]

Nanocrystalline ferrites. — With the recent advances in nanotechnology, ferrites have become again of considerable interest, as they exhibit altered magnetic behaviour, due to surface and size effects and interparticle interactions. We investigated the crystallographic properties and the magnetic ordering of some ferrites which seem to be promising for industrial applications. For **magnetite** (Fe_3O_4, Fd-3m), samples with grain sizes down to 15 nm were prepared: the different dependency of the magnetisation of the two ferrimagnetically coupled sublattices and slight changes of the first neighbour Fe-O distances could be established. The atomic coordinates and the vacancy distribution in nanocrystalline needle shaped **maghemite** (γ-Fe_2O_3) particles, with average size 240 × 30 nm, were determined in space group $P4_12_12$. The influence of the grain size, in the range of 10nm-1μm, on the local atomic and magnetic parameters of $BaFe_{12-2x}(CoTi)_{2x}O_{19}$, (x=0.45 – 1) **hexaferrites** was also revealed.

Soft magnetic alloys. — The macro- and mesoscopic magnetic properties, as a function of temperature and external magnetic field, of the nanocrystalline soft-magnetic alloy **$Fe_{73.5}Nb_3Cu_1Si_{13.5}B_9$** have been investigated by using the 3D neutron depolarisation technique. Isothermal hysteresis measurements and temperature scans at fixed external fields have been carried out in the temperature range from room temperature up to T = 623 K and in magnetic fields up to H = 24 A/cm. Isothermal hysteresis measurements with a magnetic field applied along the long axis of the 24 μm thick ribbon showed an anomalous temperature dependence. The deduced coercive force as a function of temperature shows a pre-peak around T ≈ 550 K, just below the Curie temperature of the amorphous matrix at T_C = 575 K, where the material looses its soft magnetic properties. At weaker fields, the inherent magnetic anisotropy of the ribbon dominates the external field and an alternating up-down domain structure perpendicular to the long axis of the ribbon develops. This structure saturates approximately at the reverse coercive field (H ≈ $-H_c$) where the sample magnetisation vanishes. The temperature dependence of the saturation magnetization of the z-domains (B_Z) is shown in Fig. 1.a. Temperature scans at different external fields showed an unexpected, non-monotonic evolution of the sample magnetisation B = μ_oM, exhibiting a sudden increase in the magnetisation above T ≈ 530 K and a local maximum at T ≈ 540 K (see Fig.1.b). For the explanation of this feature, a model implying a change in the magnetic coupling between amorphous and nanocrystalline phases close to the Curie temperature of the amorphous matrix is proposed.

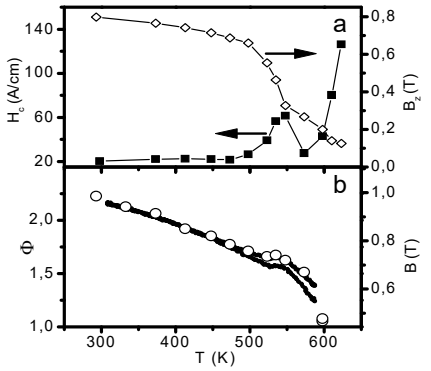

Figure 1. (a) Sample coercivity H_c and the average magnetic induction of the alternating up-down z domains, (b) Polarisation rotation Φ and the magnetic induction of the sample. Circles indicate the magnetisations calculated from the constant temperature hysteresis measurements.

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Liquid and amorphous systems. — A model investigation was conducted for exploring further potentialities of the Reverse Monte Carlo (RMC) technique: its possible application for determining the structural features of **dimerising associating fluids** was investigated in detail. For the purpose, molecular dynamics (MD) simulations of mixtures of monomers and dimers (at several thermodynamical conditions) have been performed. Results of MD simulations (in terms of the pair correlation function and the structure factor) have then been considered as 'experimental input' for RMC modelling. It was demonstrated that under certain conditions (at liquid-like densities), reasonable estimates for the equilibrium concentrations of a simple dimerisation reaction can be derived. It is also worth noting that partial (monomer dimer, dimer-dimer and monomer-monomer) pair correlation functions have also been obtained with good accuracy.

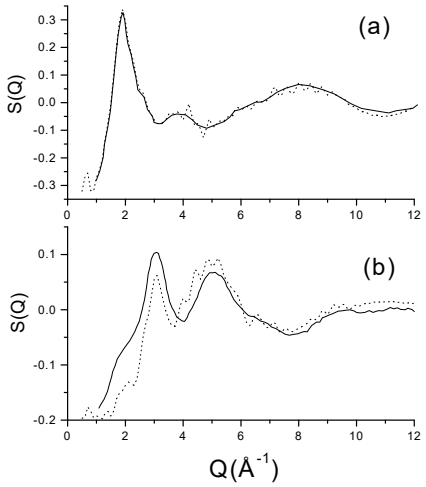

Figure 2 (a) Total neutron structure factors for D_2O. Solid line: neutron diffraction from 1997; dashed line: reconstructed from the partial pair correlation functions derived by RMC. (b) Total neutron structure factors for H_2O. Solid line: neutron diffraction from 1997; dashed line: reconstructed from the partial pair correlation functions derived by RMC.

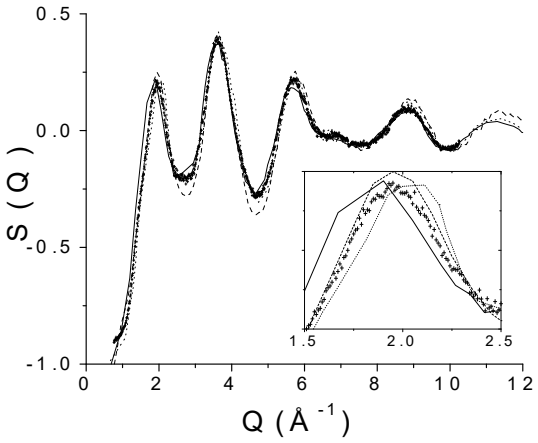

Figure 3. Experimental structure factors of amorphous selenium. Solid line: X-ray diffraction from 1968; dashed line: neutron diffraction (ND) from 1975; dots: ND from 1982; crosses: present ND measurement. The inset shows the environment of the first maximum, between 1.5 and 2.5 $Å^{-1}$. (Note that the small fluctuations on the curve corresponding to the present study are characteristic to the statistical error of the measurement.)

Continuing our efforts towards the determination of reliable partial pair correlation functions of **liquid water**, a new set of RMC calculations have been made concerning the substance. It has been shown that the consistency between partial pair correlation functions obtained by RMC and neutron diffraction measurements on pure H_2O is improving as these experiments are focusing more and more on the difficulties of hydrogeneous samples. However, the difference between the quality of data on pure D_2O and pure H_2O is still too large for being able to apply them simultaneously with sufficient confidence (see Fig.2).

A new neutron diffraction measurement on (ball milled) **amorphous selenium** (a-Se) has been performed. The structure factor (Fig.3) was interpreted by the RMC method and simultaneously, detailed RMC modelling was carried out on numerous earlier diffraction data taken on a-Se. Based on this comparative study, it is suggested that the material,

independently of the method of preparation, contains chain molecules of variable lengths and that the dominance of Se_8 rings is improbable.

Methodological developments - The MTEST four-circle neutron diffractometer – applicable for strain and texture measurements - has been put into operation at a thermal channel of the 10 MW Budapest reactor. The PSD neutron powder diffractometer working at the tangential channel of the reactor has been equipped with a new detector system (containing three linear position sensitive ^{3}He-detectors) .

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Grants and international cooperations

OTKA T 029402 Neutron diffraction study and modelling of partially ordered systems (E. Sváb, 1999-2002)

OTKA T 029433 Dynamic neutron-, gamma-, and x-ray radiography investigations and modelling of streaming processes (sub-contract E. Sváb, 1999-2002)

OTKA T 32308 Neutron diffraction at the Budapest Research Reactor (L. Pusztai, 2000-2003)

OTKA N 31766 Polarised neutron investigations of nanocrystalline materials (L. Pusztai, 2000-2002)

EU HPRI-CT-1999-50013 Software for computer Aided Neutron Scattering (L. Pusztai, 2000-2002)

NWO N 31766 Polarised neutron investigations of nanocrystalline materials (L. Pusztai, 2000-2003)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP8: Atomic level structural studies by photons and neutrons. (G. Faigel, 2000-2003)

AKP 2000-92,4 Interpretation of diffraction data from molecular liquids (L. Pusztai, 2001-2002)

Bilateral travel grant of the Hungarian and Bulgarian Academies of Sciences, No. 5. Structure studies by neutron diffraction (E. Sváb, 2000-2002)

Bilateral travel grant of the Hungarian Academy of Sciences and the Mexican Ministry of Science and Technology, No. 7 (L. Pusztai, 2001-2003)

Long term visitors

— Guillaume Evrard, post-doctoral fellow for 2 years starting at 01.01.2002 (Host: L. Pusztai).

— Kiril Krezhov, senior scientist from Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, November 22-December 22, 2002 (Host: E. Sváb)

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Articles

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Books, book chapters

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See also E.15.

L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, S. Varró and I. Bányász

Experimental research. — We have demonstrated experimentally (in cooperation with the Faigel-group) that the strong X-ray radiation -- observed in former experiments, where we focussed intense psec duration laser pulses onto metal surfaces kept on positive voltages consists of two components: 1. A great part of X-rays comes simultaneously with the laser pulses (time resolved detection). 2. Another contribution is emitted however, without laser from the interaction part of the surface, modified by the interaction during long time period (time integrated detection). All former published experiments have to be re-envisaged from this point of view.

Theoretical research. — We performed many-particle simulations of the quantum electron gas in a metal surface, irradiated with intense femtosecond laser pulses at grazing incidence. A gradual population of electron states is predicted, where subsequent steps of occupation probabilities are separated by the incident photon energy hν. During the laser interaction with pulses of the order of 100 fs, oscillations of the occupation of states in the energy domain are shown to appear, leading to an inversion of states in the conduction band. On the basis of the Fermi–Dirac distribution and resulting final occupations of states, an estimate of the average temperature of the conduction electrons in metal films subject to laser irradiation is given. This result furnishes a key to interprete our multiphoton resonance experiment performed some time ago, exhibiting very sharp resonance curves when the five laser photon energy coincided with the metal work function value.

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Grants and international cooperations

OTKA T032375 Experimental and theoretical investigation of new fundamental physical processes (laser-matter interactions) induced by laser beams of superintense, 10^{15}-10^{20} W/cm^2 laser systems. (Gy. Farkas, 2000-2003)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP11: Interaction of light with condensed matter (N. Éber, 2000-2003)

TéT – F-3/00 (Hungarian-French Bilateral): Application of x-ray sources in the "femtosecond" regime. (Gy. Farkas, 2001-2002)

TéT –D-41/00 (Hungarian-German Bilateral): Study of laser-induced nonlinear processes in thin solid films. (S. Varró, 2001-2002)

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L.4. Lakó S; Analytical modeling of second harmonic generation of focused femtosecond laser pulses with arbitrary spectra and spatial intensity distribution; *Laser Physics*; accepted for publication.

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L.8. Lakó S; Analytical modeling of second harmonic generation of focused femtosecond laser pulses with arbitrary spectral and spatial intensity distribution; In: Conf. Proc. *Laser Physics Workshop* (Bratislava, July 1-5 2002); p.85; accepted for publication

M. LASER PHYSICS

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

Hollow cathode lasers. — Research of hollow cathode metal ion lasers nowadays is directed toward ultraviolet transitions. In most cases these lasers are pumped through charge transfer collisions between noble gas ions and ground state metal atoms resulting in ionization and excitation of the metal atoms in a single step. The metal atom density necessary for the laser action can be achieved by two means: the metal can be evaporated or the cathode of the discharge can be sputtered by positive ions from the discharge plasma. High voltage hollow cathode discharges were developed with the aim of optimizing the parameters of sputtered constructions. We are currently investigating the possibility of the application of high voltage electrode arrangements for the purpose of heated lasers. The other direction of our current research is the extension of the lifetime of sputtered lasers.

Gas discharge and plasma research. — We have investigated the axial and radial profiles of light emission from glow discharges experimentally and by means of self-consistent computer simulation. The characteristic changes of emission profiles through the Townsend discharge – normal glow – abnormal glow transition were identified. The apparent secondary electron yield at the cathode has been determined from the simulations. In the field of strongly coupled plasmas we have studied the dynamical properties of layered systems of charged particles by molecular dynamics simulations. We have also investigated the spatial-temporal localization of particles in strongly-coupled plasmas in their liquid phase. Using a correlation technique to monitor the changes of the particles' surroundings we have proven that in the strongly-coupled liquid phase the trapping of the particles covers several plasma oscillation cycles.

Electrolyte cathode atmospheric glow discharge. — Research has been carried out to improve the capabilities of the electrolyte cathode atmospheric glow discharge (ELCAD). In the new experiments the electrolyte was flown through a narrow capillary glass tube. The electrolyte appearing at the end of the vertically placed capillary tube acted as cathode of the discharge. This is a significant difference compared to the ELCAD used up to now. In the present case the discharge has an abnormal character and a significant increase of current density could be obtained. The experimental arrangement contained a special flow injection part to inject metal atoms in the discharge. Using this apparatus we succeeded to show in a very small volume the presence of a very small amount of metal (0.5 - 1 ng of Zn, Cd, Cu, Pb, Ni). This capillary - ELCAD arrangement gives a possibility to indicate the presence of metal concentrations of an order of magnitude smaller than that in the conventional ELCAD, which result is important in view of the construction of measuring devices for environmental protection.

Ellipsometry. — We have developed a special “Tricolor” laser system for the imaging spectroellipsometer. The computer controlled unit nearly homogeneously illuminates the samples at different wavelengths: 530nm, 670nm and 781nm simultaneously, resulting multispectral ellipsometric data for fast, real time quality control of large (up to 5”) semiconductor surfaces.

Optogalvanic effect. — In the optogalvanic effect (OGE) a gas discharge is irradiated with a light beam (usually a laser), the wavelength being resonant with a transition of the gas

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atoms in the discharge. The absorption of this light can change the ionization state in the discharge , tube voltage can increase (negative OGE), or it can decrease (positive OGE). It has been observed in the central region of He, Ne and Ar hollow cathode discharges that in the 5 – 10 mbar pressure range a change of the sign of the OGE occurs, by increasing the pressure it changes from positive to negative. We have developed a model in order to explain this phenomenon. In the model the ions in the discharge are assumed to be produced by electron excitation from the ground and metastable states. The ion loss is assumed to be a result of diffusion out of the discharge volume and three body recombination of ions. Consideration of results of the model show that within discharge conditions when diffusion is the dominant loss the OGE is positive, while when recombination becomes the dominant loss the OGE changes sign to negative.

Spectroscopy. — On the basis of available experimental and theoretical data the role of Stark effect in the homogeneous line broadening of the green and blue laser lines in a hollow cathode He-Cd^+ laser discharge was studied. It was found, that as the electron density in HC laser plasmas can be two orders of magnitude larger, than that in the positive column of a glow discharge, Stark broadening in HC lasers can give a significant contribution to the homogeneous line-width. Its actual role, however, depends on the properties of the atomic or ionic levels involved. It was shown, that at typical laser discharge parameters, for the 538 nm line the Stark line-width is comparable with the pressure broadened natural line-width, while for the 442 nm line both are significantly smaller. The increased homogeneous line-width results in single mode operation for the green line - as it was observed earlier - while for the blue one it does not.

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Grants and international cooperations

NATO SfP 971989 High beam quality UV lasers for microelectronics (K. Rózsa, 1999-2004)

OMFB 01553/99 High beam quality UV lasers for microelectronics (K. Rózsa, 1999-2004)

OTKA T – 25941 Ultraviolet lasers in controllable-temperature hollow cathode discharges (K. Rózsa, 1998-2002)

OTKA T - 34156 Modern plasma simulation techniques (Z. Donkó, 2001-2004)

MTA-OTKA-NSF 28 Strongly coupled Coulomb systems (Z. Donkó, 2001-2003)

OTKA T- 29112 Excitation processes in electrolyte cathode glow discharge (P. Mezei , 1999-2002)

OMFB IKTA-2000 Digital imaging spectroellypsometrical quality control arrangement (Z.GY. Horváth, 2001-2004)

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Articles

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N. METAL OPTICS

Z. Szentirmay, A. Hoffmann, N. Kroó, Z. Lenkefi

Construction of a novel scanning tunnell microscope (STM). — In cooperation with the STM group of the Max Planck Institute for Quantum Optics in Munich (Germany) a new type of STM was constructed which is recently tested. The fundamental observation which lead to the construction was that if one applied a laser illumination of the metallic sample in ATR (i.e. attenuated total reflection) geometry, the electric signal measured on the tip contains components which are characteristic for i) the surface plasmon field and ii) the thermal behaviour (Seebeck potential and thermal dilatation) of the sample. As usual, the thermal signal has the slowest rise up in time.

The instrument is realized using a boxcar integrator with three time gates. The first gate is open for 15 μs after the rise up of the 50 μs long laser pulse (plasmon signal). The second gate opens 15 μs after the decay of laser signal and is open for 15 μs (thermal channel). The third gate measures the background with 45 μs before the laser signal (reference channel). The content of this channel is subtracted automatically from that of the other channels. Naturally, the conventional topographic picture is also made simultaneously with the plasmon (Ch.1) and thermal (Ch.2) pictures.

In order to estimate experimentally the contribution of the plasmon and thermal components to the detected images, measurements were made on 50 nm thick (semitransparent) silver and gold metal films using the excitation from a diode laser of 670 nm wavelength, chopped electronically with 1.8 kHz frequency. Measurements were performed using W, Ag and Ag tips in order to distinguish between the Seebeck potential and other thermal constituents.

The observations showed that in the case when the tip and film were made from similar metals (e.g. gold tip and gold layer etc,) the thermal components are smaller than in other cases (as e.g. tungsten tip and gold layer). Consequently, STM measurements are in this case material dependent.

This effect was clearly demonstrated using gold films with laser evaporated thin (0.5 – 2 nm) silver overlayer. The silver was evaporated in the form of high velocity clusters generating craters in the soft gold basis layer (Fig.1). In the center of craters always expected a more or less buried silver particle or cluster, which has been detected in the plasmon and thermal pictures simultaneously.

Further testings of the instrument are in progress.

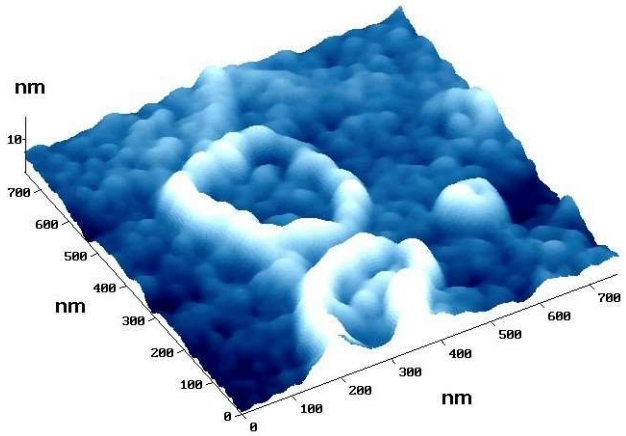

Fig.1. Craters formed in a 50 nm thick gold layer by laser sputtering of silver overlayer. Average silver thickness: 1.6 nm. (An AFM image.)

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Grants and international cooperations

OM 00224/2001 Szechenyi NRP "Nanotechnology" (Participant: Zs. Szentirmai, 2001-2003)

OM 005/2001 Szechenyi NKFP "Enviromental pollution and aerosols." (Participant: Zs. Szentirmai, 2000-2002)

Max Planck Institute for Quantum Optics (Garching, Germany): Surface plasmon research using STM (H. Walther, N,Kroó, continuous)

Physical Institute of University of Bonn (Germany): Charge density waves in photorefractive materials (Á. Hoffmann, 2000-2003)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP11: Interaction of light with condensed matter. (N. Éber, 2000-2003)

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Articles

N.1. Szentirmay Z, Kroó N; Preparation of silver tips for surface plasmon microscopy; *Rev. Sci. Instr.*; accepted for publication

Articles in Hungarian

N.2. Szentirmay Zs, Czitrovszky A, Jani P; A porszennyezettség méret szerinti eloszlásának vizsgálata a Pilisben (Determination of size distribution of airborne dust particles in the Pilis mountain, in Hungarian); *Egészségtudomány*; **46**, 60-66, (2002).

O. LASER APPLICATION

A. Czitrovszky, M. Füle[#], P. Jani, I. Kertész, Á. Kiss, M. Koós, S. Lakó[#], Z. Lipp[#], A. Nagy, D. Oszetzky, I. Pócsik, S. Tóth[#], M. Veres[#]

Optical measuring techniques. — A new dual wavelength forward-backward scattering laser particle measurement method was developed for sizing, counting and estimation of the complex refractive index of aerosol particles in the sub-micron and micron size-range in collaboration with Vienna University. The modeling of this method was performed for different particles using a new algorithm. A measuring head with two different lasers (green and red), and four detectors (forward and backward scattering for both wavelengths) was constructed and elaborated. The assembling of the measuring head was finished and preliminary testing was started. A new nuclear airborne particle counter with a modular measuring head was tested. In the frame of EU COLOSS program (measurement of the hot nuclear aerosols released from LWR fuel rods heated up to 2200°C) the previously measured data were analyzed.

The mechanical and electronic system of the previously developed Differential Mobility Analyzer was tested.

In the frame of *NRDP Atmospheric Pollution of the Atmosphere*, a mobile laboratory installed in a FIAT DUCATO microbus (Fig.1) was developed for environmental monitoring of atmospheric aerosols and measurement of air contamination within the big cities. The laboratory is equipped with different airborne and liquidborne particle counters, cascade impactors, air samplers, and devices for the measurement of meteorological conditions (wind velocity, wind direction, temperature, humidity, etc.)

Fig.1

Mobile laboratory for investigation of atmospheric aerosols.

The measuring system for the standardles determination of the quantum efficiency of the photon counting detectors using entangled photon pairs was reconstructed.

In the frame of the *NRDP Nanotechnology* project photon correlation experiments and system development for the simultaneous size and velocity measurement of nanometer size particles were continued. Development of integrated optical elements using frequency

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stabilized semiconductor lasers, fiber optical light guides and avalanche photodiodes is currently under test for system optimization.

Development of measuring techniques based on statistical properties of scattered light on ensemble of aerosol particles is in progress. A *picosecond* time resolution measuring system is tested. Numerical simulation of scattering statistics on ensemble of aerosol particles was performed.

Amorphous carbon layers. — Our research work was focused onto carbon based amorphous materials. Various forms of amorphous carbon - diamond-like (DLC), polymeric soft material, nitrogenated layers, etc. - have unique properties, which are important from the point of view of application. DLC layers have been prepared by pulsed laser deposition (PLD) method in which the graphite target was ablated by ultraviolet excimer lasers (ArF: 193 nm, 18 ns; XeCl : 308 nm, 30 ns) in vacuum or methane ambient of different pressure. Nano-structural properties and electronic levels near band edges of the thin amorphous carbon layers were studied with the aim to find correlation between π electron density of states and atomic bonding structure.

A new discovery was, that in a given range of gas pressure and deposition voltage by using the radio-frequency enhanced chemical vapor deposition (*rf*-CVD) system beside the deposition of amorphous carbon film onto the substrate, amorphous carbon nano-particles were also prepared. These particles are spherical, and show a narrow size-distribution around 100 nm. In this size range the particles in the plasma agglomerate into necklace-like chains and sediment in the ground plate of the chamber. On the driven electrode a solid film forms, with intensive contribution of these particles. The atomic force microscopic picture of this film surface show a cauliflower-like structure (Fig. 2), proving, that these particles reached the sample holder separately, before their chain-like aggregation.

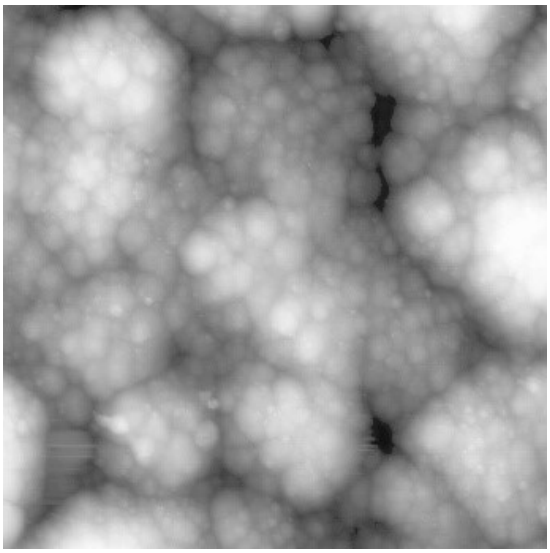

Fig. 2.

Atomic force microscopic (AFM) picture of the amorphous carbon clusters deposited on the substrate, where the clusters contribute to the formation of an amorphous carbon film. The real size of the whole picture is 5 μm x 5 μm

Detailed study of these nano-particles is in progress. Raman and infrared spectroscopy and photoluminescence investigations are used to study the properties of these materials. It is a unique possibility to study an amorphous solid film, and the system of nano-clusters, from which the film was formed. The spectral features of the clusters are narrow, showing the naturally expected stress free conditions, and the spectra of the solid film contain broader, more overlapping bands, as a consequence of the spatial repulsion of the clusters, and the impact of the high energy ions, which are bombarding the surface of the forming films.

The amorphous carbon based electronics have the general problem of unsolved doping. The best candidate element for doping is nitrogen, however, nitrogen can be incorporated in

relatively small quantity only into the amorphous carbon layer. It is not clear yet in the literature, whether a real doping process takes place, or just a clustering of the nitrogenated sites is able to explain the measured data. For further understanding of this problem we have prepared a series of nitrogenated samples within the possible range of nitrogen content. Our Raman scattering and photoluminescence measurements show new features, which support the doping interpretation of the processes.

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Grants and international cooperations

OM-NATO-00006-2000 Energy storage possibilities in nano-composites (I. Pócsik, 2002-2004)

NATO SfP-976913 Carbon Based Storage (I. Pócsik, 2000-2004)

Hungarian-Greek Intergovernmental S & T Cooperation Programme (I. Pócsik, GR-31 2002-03)

Hungarian-Ukrainian Intergovernmental S & T Cooperation Programme (I. Pócsik UK-6/2003-04)

Bilateral Austro-Hungarian Cooperation, Contract No A-20/01 (A. Czitrovszky, 2002-2004)

Military Technical Project 422/2001, (P. Jani, 2001-2002)

National Research and Development Program NKFP-005/2000, Environmental Pollution of the Atmosphere (coordinator: A. Czitrovszky, 2001-2004)

National Researh and Development Program, NKFP 064/2000, Nanotechnology (sub-coordinator: A. Czitrovszky, 2001-2004)

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See also L.4., L.8., P.2., P.3., P.4.

P. FEMTOSECOND LASERS

R. Szipőcs, Á. Bányász[#], K. Szőcs

Optical thin-films in femtosecond laser systems. — Continuing our research started in 1993, dispersive dielectric mirrors were developed for different femtosecond laser systems such as: (a) ion-beam-sputtered (IBS) multi-cavity Gires-Tournois mirrors (MCGTI) for mode-locked, mirror-dispersion-controlled, diode pumped Cr:LISAF lasers operating at University of St. Andrews and ICS Trieste and (b) ultrabroadband chirped mirrors (CM) for optical parametric amplifiers (OPA) in collaboration with R&D Lézer-Optika Bt., Hungary, and MLD Technologies, USA. The MCGTI mirrors exhibit reflectivities R > 99.97% and negative group delay dispersion of -100 ± 10 fs^2 over a bandwidth of 780 to 880 nm. Dispersive properties of MCGTI mirrors originate from coupled resonances in multiple λ/2 cavities embedded in the layer structure. Alternatively, the design of our ultrabroadband CM-s developed for the OPA system was obtained by our spatial frequency domain optimization technique. The mirrors exhibit high reflectivity and a constant group delay dispersion over 210 THz and 140 THz, respectively, supporting tunable 7 fs pulses in the visible optical parametric amplifier system built at the University of Toronto.

Pulse compression in microstructure (photonic crystal) optical fibers. — In collaboration with OFS Fitel Laboratory (USA), and researchers from SZTE (Szeged, Hungary) and R&D Lézer-Optika Bt., the possibility of femtosecond pulse compression in microstructure optical fibers were investigated both theoretically and experimentally. Femtosecond pulses with energies of 1 nJ and time durations of 150 fs from our tunable, 76 MHz Ti:sapphire laser oscillator operating at around 750 nm were used for our studies. The length of the pulses can be compressed to one tenth by applying our high delta, single mode microstructure optical fiber exhibiting zero group delay dispersion at 767 nm, and by proper extracavity dispersion compensation (Fig.1). Our experimental results fit well to computer simulation results, which are based on our theoretical model developed for describing the nonlinear pulse propagation in the optical fiber. The model comprises the reduced form of the differential equation that worked correctly for modeling fs pulse optical parametric oscillators. We are convinced that our proposed simple "upgrade" for 100 fs pulse laser oscillators will help to considerably reduce the temporal resolution of ultrafast measurements in many ultrafast spectroscopy laboratories.

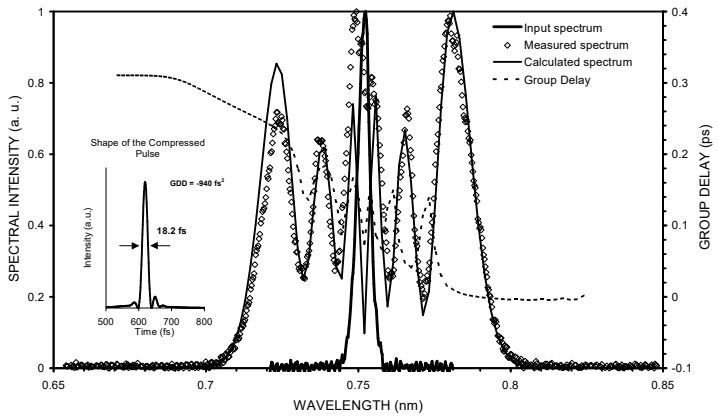

Fig.1 150 fs to 18 fs pulse compression by a microstructure optical fiber and dispersion compensation

[#] Ph.D. student

Femtosecond time resolved spectroscopy using a pump-probe setup. — In collaboration with OFS Fitel Laboratory, USA and Dept. of Physical Chemistry of ELTE University, a femtosecond pump-probe experimental setup has been developed for time resolved spectroscopy on chemical, biological and medical samples. The setup comprises a synchronous viola/blue pump pulse for excitation and a white light continuum probe pulse for transient absorption measurements over the 450..1100 nm wavelength regime. The tunable 100 fs pumpe pulses are obtained by second-harmonic-generation of our tunable 100 fs NIR pulses generated by our FemtoRose 100 TUN Ti:sapphire oscillator in a BBO crystal. The continuum is generated in a relatively long (ca. 12 cm long) piece of special microstructure optical fiber drawn by OFS Fitel Laboratory, USA. The setup is supplied with Windows 98 based software automatically setting system parameters such as the time delay between the pump and probe pulses, pump and probe wavelengths, voltage on the PMT, chopper frequency, slit width of the monochromator, etc., and collecting measured data through a data acquisition card (Fig.2).

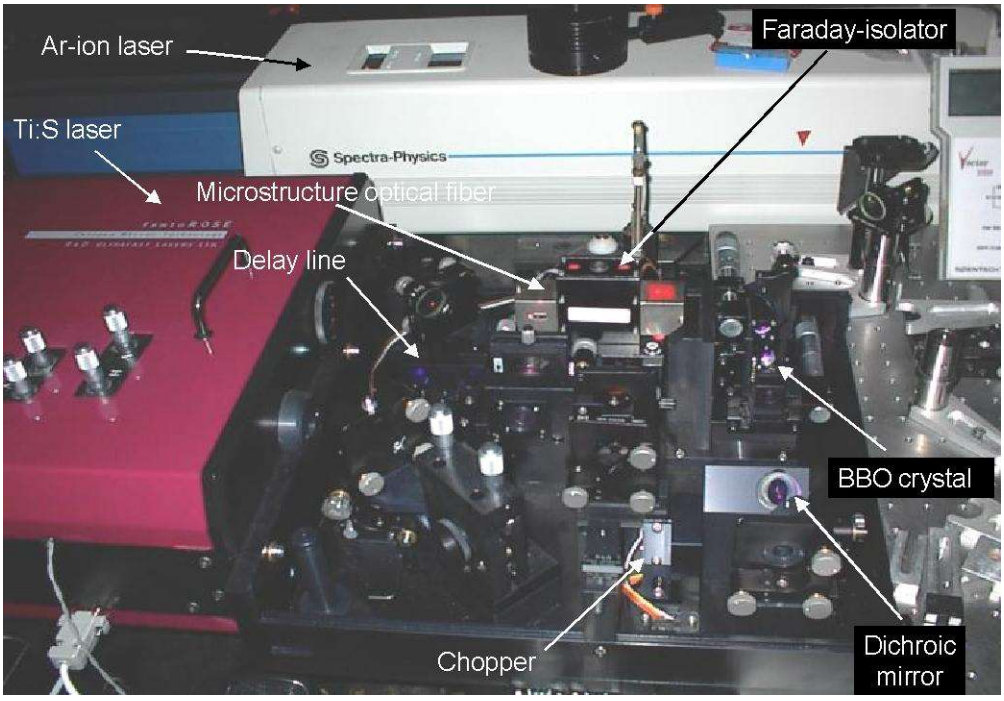

Fig. 2 A femtosecond pulse pump/probe setup developed for transient absorption measurements

Sub-micrometer pulse train machining of diamond like carbon layers. — We fabricated sub-micrometer holes on 100 nm diamond like amorphous carbon (DLC) coated surfaces by ablation with femtosecond laser pulse trains of a Ti:sapphire laser oscillator. In the case of DLC coating on Si wafer, one order of magnitude less than the focal spot, sub-micrometer damaged area could be achieved due to nonlinear processes.

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Publications

Articles

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Q. OPTICAL THIN FILMS

K. Ferencz

Optical thin film structures consisting of nanoscale laminated layers. — We have started intensive research concerning the development of optical thin film structures containing of nanooptically thick layers for advanced applications in laser physics and information technology. We have developed a new electron-beam deposition technology for producing of optical coatings containing nanooptically thick titania, silica, tantala, alumina and silver layers. Using needle-like optimization thin film design method, we have successfully produced nanooptical nonpolarizing beam-splitters, dichroic filters, heat protecting filters, antireflection coatings, non-reflecting attenuation, nonpolarizing high-reflectors for wide band of angles of incidences, polarizing beam splitters, etc. Our polarizing beam-splitter cubes have better than 1000 : 1 extinction ratio, if the material is BK7 optical glass, the high-index material is TiO_2 or Ta_2O_5, the low-index material is SiO_2, at laser wavelengths of 635, 532 or 405 nm.

Other developments on optical coatings. — Our work on ultrafast optical coatings is still in progress co-operating with the Institute of Photonics at the Technical University of Vienna, Austria (Prof. Ferenc Krausz) for many types of advanced applications in laser oscillators, amplifiers, autocorrelators, coherent X-ray generation, etc. We have successfully developed new type of coatings for tilted-front-interface chirped mirror technique, as a new mode for the reduction of the fluctuations of the group delay dispersion of the conventional chirped mirrors, which opens the way for the construction of laser oscillators emitting shorter than 5 fs pulses.

We have continued the development of integrated optical grating couplers for biotechnological application as a switching or sensing element using bacteriorhodopsine as non-linear optical material. Using our waveguide structures a direct optical switching effect was successfully detected in co-operation with the Biophysics Institute of the Szeged Biological Research Centre (Prof. Pál Ormos). New types of interference filters were also developed for high sensitivity detection of protein molecules elaborated by gene manipulation methods.

These results were obtained in the frame of the scientific co-operation between the Institute and Optilab Ltd.

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Contract

OPTILAB-SZFKI No. 201/2002
OPTILAB-SZFKI No. 203/2002

Grants and international cooperations

OMFB-02432/2000 Nanobiotechnological devices based on bacteriorhodopsin (K. Ferencz, 2000-2002)

NATO SfP 974262 Optoelectronic Devices Based on the Protein Bacteriorhodopsin (Coordinator: P. Ormos*, participant: K. Ferencz, 2000-2004)

NKFP3/064/2001 Széchenyi NRP: Nanotechnology (A. Czitrovszky, participant: K. ferencz, 2001-2004)

EU CRAFT, Contract No. QLKG-CT-2002-70549 Ultrahigh resolution opthalmologic optical coherence tomography (Coordinator: A. Stingl*, Austria, participant: K. Ferencz, 2002-2004)

NKFP3A/0005/2002 Nanobiotechnology: Elaborate a method to build nanotechnological devices for use in biology (Coordinator: P. Ormos*, participant: K. Ferencz, 2002-2005)

R. GROWTH AND CHARACTERIZATION OF OPTICAL CRYSTALS

I. Földvári, L. Bencs, E. Beregi, V. Horváth, Á. Péter, K. Polgár, O. Szakács, Zs. Szaller

Growth and study of nonlinear borate crystals – Chromium doped $YAl_3(BO_3)_4$ (YAB) single crystals were grown by the top-seeded flux method. Cr:YAB is a prospective self-frequency-doubling laser material. The excitation and emission spectra of Cr^{3+} were determined. The luminescence spectrum at RT consists of a sharp doublet (R lines, $^2E - {}^4A_2$ transition) and a broad band at higher energies ($^4T_2 - {}^4A_2$ transition). At low temperatures the R_1 emission line becomes dominant. The thermal shift of its position is due to phonon coupling (300 cm^{-1} average phonon energy). The chromium is situated in the Al-sites of the crystal, that represents strong, octahedral crystal field, characterized by the Dq = 1662 cm^{-1} crystal field, and the B = 684 cm^{-1} and C = 3194 cm^{-1} Racah parameters. The configuration coordinate diagram of Cr^{3+} ion in YAB was calculated from the spectral data and the lifetime of the excited state in the Born-Oppenheimer approximation. The model used considers spin-orbit coupling of the ^2E and $^4T_2$ states, and a coupling constant of 140 cm^{-1} was determined by fitting.

Growth and study of stoichiometric $LiNbO_3$ single crystals – The phase diagram of the K_2O—Li_2O—Nb_2O_5 ternary system was determined along the $LiNbO_3$—K_2O line up to 20 mole % of K_2O. The thermo-analitical measurements were completed by crystal growth experiments. In this range Li_3NbO_4, $LiNbO_3$, $K_3Li_2Nb_5O_{15}$ and $KNbO_3$ phases were identified by X-ray diffraction. The real composition of the crystals was checked by the absorption edge shift method, and it was shown that stoichiometric $LiNbO_3$ crystals can only be grown if the flux composition is between 13.8 and 18 mole % of K_2O. These observations were used to optimize the top-seeded flux method for growing stoichiometric $LiNbO_3$, and 0.4999 Li / Li+Nb ratio was achieved.

By the Z-scan method light-induced refractive index change and nonlinear absorption were determined in undoped and Mg-doped $LiNbO_3$ crystals with congruent and stoichiometric composition, using Ar-ion laser up to the MW/cm^2 level. In the 5 mole% Mg-doped stoichiometric crystals a positive extraordinary refractive index change was observed ($\Delta n_e=2.5\times10^{-5}$ at 0.37 MW/cm^2 light intensity), opposite to all the other samples, including the Mg-doped congruent and the undoped stoichiometric crystals where $\Delta n_e<0$. At the same conditions, the measured $|\Delta n_e|$ values with 5 mole% Mg-doping level were 20 times smaller for the stoichiometric crystals than for the congruent ones. Accordingly, the previously observed laser resistance of the Mg-doped crystal can be improved by proper combination of shifted composition and Mg-dopant.

Growth and study of TeO_2 and bismuth tellurite crystals – Bi_2TeO_5 and TeO_2 single crystals were grown by the Czohralski technique. The oxidation kinetics of Bi_2TeO_5 was investigated by thermogravimetric experiments, combining non-isothermal (1–10°C/min) and isothermal (600–700°C) sections, at oxygen partial pressures of 21-101 kPa. The kinetic model contained an empirical $f(\alpha)$ function to describe the dependence of the reaction rate on the reacted fraction (α). The unknown parameters were determined by the least-squares evaluation of 12 different experiments with baseline correction. The low activation energy values obtained (35–39kJ/mole) indicate that the rate limiting factors are connected to diffusion and other physical processes with moderate temperature dependence. The analysis of the $f(\alpha)$ functions revealed a complex kinetic behavior influenced by the diffusion of oxygen through the formed products and the accelerating effect of internal surfaces.

Monotonously decreasing f(α) functions were observed in two different cases: (i) at T(isothermal) of 600–650°C; (ii) at oxygen partial pressures below ~ 50 kPa. Experimental conditions leading to relatively high reaction rates (at T > 650°C and P_{O_2} above ~ 50 kPa) favor f(α) functions starting with an increasing section and reaching a maximum around $\alpha \approx 0.3–0.5$. Non-isothermal experimental conditions also led to similar f(α).

The Er lattice position in Bi_2TeO_5:Er single crystals was followed by nuclear techniques using 2.7 MeV He^+ ions. Due to the large portion of heavy Bi ions in the crystal, the Rutherford backscattering (RBS) technique was not satisfactory, but despite of the complex crystal structure, the PIXE/channeling working configuration was able to locate the Er^{3+} ions in the different Bi sites. This confirms the previous assumptions based on the optical spectra.

The TeO_2 crystals were irradiated by Xe, Kr, Ar, Ne and O ions in the energy range of 0.35—2.3 MeV. The track evolutions in the crystals were followed by RBS in channeling geometry. No damage was observed using O ions, while the other ions induced 6—16 nm diameter tracks. The linear $R(e)^2$ - S_e track evolution curve (where R(e) is the effective track radius and S_e is the electronic stopping power) is in agreement with the Szenes model prediction for the ions investigated.

Analytical spectroscopic investigation of oxide and borate crystals – Flame atomic absorption spectrometric (FAAS) and inductively coupled plasma optical emission spectrometric (ICP-OES) methods were developed for reliable determination of the constituents of YAB single crystals. The possible matrix effects were studied at various compositions of sample solutions. The mixtures of Cs- and La-chlorides as spectrochemical buffers were proved to be the most accurate and precise in the for FAAS measurements.

In the analysis of Co, Mn and Ni dopant levels in Bi_2TeO_5 crystals we observed the flattening of the calibration curves when the transversally heated graphite atomizer (THGA) was used with standard acidic solutions. This phenomenon is attributed to the loss of sample vapors from the THGA furnace at its ends. By the proper alteration of the atomization conditions (i.e. using either chemical modifiers or the mini-flow of the internal furnace gas during atomization, or the end capped graphite tubes) we could minimize the vapor loss and improve the linearity of the calibration curves.

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Grants and international cooperations

OTKA T-034176	Preparation and investigation of nonlinear optical crystals and crystal structures (K. Polgár, 2001-4)
OTKA T-032339	Optimization of the parameters of the acousto-optic tunable filters (L. Jakab (BME) and Á. Péter, 2000-2003)

OTKA T-029756 Growth and complex study of bismuth tellurite single crystals (I. Földvári, 1999-2002)

OTKA T038017 Development of laser ablation and electrothermal sample introduction methods for the atom spectrochemical study of element distributions (T. Kántor, (ELTE) and L. Bencs, 2002-2005)

Hungarian Széchenyi National Scientific Research Fund (NSRF) OM Grant No. 224/2001 Nanotechnology: Nonlinear crystals (J. Gyulai (MTA MFA) and Á. Péter, 2001-4)

Hungarian Ministry of Education Research Program, OM-DDKKK 00004/2000 (I. Sántha (PTE) and Á. Péter, 2001-3).

Hungarian Ministry of Education Research Project, OM FKFP 30/2000. Investigation of the formation process of complex rare-earth borates by thermoanalytical and X-ray diffraction methods. (J. Madarász (BME) and E. Beregi, 2000-2002)

Hungarian-German R&D project: Improvement of the analog volume holographic recording technique (I. Földvári, 2000-2002)

COST Action P8. Materials and Systems for Optical Data Storage and Processing (H.- J. Eichler (Berlin) and I. Földvári, 2002-5)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP12: Growth and complex study of optical crystals (J. Janszky)

Long term visitor

— Rebeca Sosa F., Universidad Autonoma Metropolitana, Iztapalpa, Mexico, D.F., October 2002, 1 year, (Host: I. Földvári)

Publications:

Articles

R.1. Dominiak-Dzik G*, Ryba-Romanowski W*, Grinberg M*, Beregi E, Kovács L; Excited-state relaxation dynamics of Cr^{3+} in $YAl_3(BO_3)_4$; *J Phys Condens Matter*; **14**, 5229-37, (2002)

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R.4. Polgár K, Péter Á, Földvári I; Crystal growth and stoichiometry of $LiNbO_3$ prepared by flux method; *Opt Mater*; **19**, 7-11, (2002)

R.5. Polgár K, Péter Á, Pöppl L*, Ferriol M*, Földvári I; Chemical and thermal conditions for the formation of stoichiometric $LiNbO_3$; *J Crystal Growth*; **237-239,** 682-86, (2002)

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R.12. Dierolf V*, Sandman C*, Gopalan V*, Kim S*, Polgár K; Rearrangement of rare earth defects under domain inversion in $LiNbO_3$; *Rad Eff & Def Sol*; accepted for publication

R.13. Klein RS*, Kugel GE*, Maillard A*, Polgár K, Péter Á; Absolute non-linear optical coefficients of $LiNbO_3$ for near stoichiometric crystal compositions; *Opt Mater*; accepted for publication

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R.15. Földvári I, Denz C*, Berger G*, Péter Á; Holographic performance of photorefractive Bi_2TeO_5 crystals; *Rad Eff & Def Sol*; accepted for publication

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R.18. Kukhtarev N*, Kukhtareva T*, Edwards V*, Mager L*, Fort A*, Rbino M*, Földvári I, Frazier D*, Penn B*, Abdeldayem H*, Hudson T*; Volume and surface phase holographic gratings in the photorefractive crystals. In: *Proc. 4th Annual Meeting of the COST Action P2, Application of Nonlinear Optical Phenomena and Workshop on $LiNbO_3$, Budapest 16-19 May, 2001;* Ed: Lion Y, European Commission, COST Directorate, Brussels; pp 78-84, (2002)

Others

R.19. Földvári I; Tarján Imre, Optikai egykristályok növesztése (Imre Tarján, Growth of optical single crystals, in Hungarian); *Emlékbeszédek az MTA Elhunyt tagjai felett,* Ed: Glatz Ferenc, Magyar Tudományos Akadémia, Budapest; pp. 1-16 (2002)

See also S.4., S.6., S.8., S.10., S.13., S.16., S.17., S.18., S.20.

S. CHARACTERIZATION AND POINT DEFECT STUDIES OF OPTICAL CRYSTALS

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

Characterization of optical crystals. — The dc conductivity of $CsLiB_6O_{10}$ crystals has been measured for the first time. It varies nine orders of magnitude from 50 ºC up to 750 ºC. The anisotropy of the dc conductivity of the crystals is small. The annealing of the crystals enhances their conductivity owing to the reduction of the built-in crystal water. The crystal composition has smaller effect on the electrical conductivity.

Microscopy of as-grown block structure of $YAl_3(BO_3)_4$ (YAB) crystals. — The undoped and doped YAB single crystals grown from high temperature melt solutions typically consisted of oriented rhombohedron-like macroscopic blocks of mm scales shown by optical and scanning electron microscopy. Blocks considerably influence on the quality of crystals. The characteristic block size distributions were measured in undoped and doped (Nd, Cr, Yb and V) crystals and no significant difference was found. Consequently, in the formation of the block structure the flux solvent as a major impurity may play dominant role rather than the different dopants.

Point defects in oxide crystals. — The angular variation of the single-line EPR spectrum in $YAl_3(BO_3)_4$:Ce single crystal shows axial symmetry and refers to a spin-½ defect. This indicates that the spectrum is due to Ce^{3+} ions and it substitutes for Y^{3+}. Fitting the EPR angular variations the corresponding $\mathbf{g}$ tensor principal values are determined. The EPR line width broadens and the intensity decreases with increasing temperature due to an Orbach process. The curve can be fitted with an exponential, where the activation energy is equal to 270 ± 16 cm^{-1}. This indicates that the ground state $^2F_{5/2}$ splits and the second level is 270 cm^{-1} higher than the first one.

Electron irradiation of a α-TeO_2 single crystal followed by 365-nm UV illumination at 10 K produces a new spin-½ paramagnetic center with C_2 symmetry like the Te lattice sites. Hyperfine interactions with ^{125}Te nuclei are prominent and indicate the diffuse nature of the defect's spin density. The model suggested here for the new center is a self-trapped electron and it is denoted as TeO_2'.

Composition dependent radiation induced optical absorption and luminescence of $LiNbO_3$ in the near stoichiometric region has been shown to be strongly affected by long-lived intrinsic Nb^{4+} polarons. Charge transfer processes involving polaronic states and trapping at transition metal dopants or impurities have recently been characterized also in thermochemically reduced $LiNbO_3$ crystals of various compositions in order to understand the strongly enhanced holographic storage properties observed for some of these systems.

Infrared spectroscopy of hydroxyl ions in oxide crystals. — High resolution FTIR spectroscopy was applied to $KTiOPO_4$ single crystals doped with Er or W. Vibrational transitions due to the impurity-OH defect interaction have been detected and studied. The orientation of the OH dipole along the Ti-O-Ti chains has been established with the presence of tetravalent tungsten at the Ti2 site. Thermally induced line broadening and shifts were analyzed according to the model of single phonon coupling.

The evaluation of the IR spectroscopic results on the kinetics of OH^- ions in $LiNbO_3$ cystals has been continued and improved. The isosbestic point method was used to determine more

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precisely the activation energy of OH ions in nearly stoichiometric crystals (1.05 eV ± 0.05 eV). Moreover, the difference between the ground state energies of the stable (congruent) and metastable (stoichiometric) bands was found to be about 0.07 eV.

Correlation has been observed between the experimentally determined harmonic frequencies, ω, and the anharmonicity coefficients, X, of OH bond stretching vibrations in crystalline materials. It has been shown that simple second-order perturbation approximation formulas of ω and X can explain the ω-X correlation, and they can be used to obtain the shape of the stretching potential and an estimate of the equilibrium length of an OH bond in crystalline environment.

Thermal fixing and spatial distribution of wave mixing holograms in $LiNbO_3$. — The activation energy of the thermal fixing of holographic gratings in congruent and nearly stoichiometric $LiNbO_3$ and its determination methods have been compared. Discrepancies in case of iron dopant for the holographic scattering and two-wave mixing methods were observed. One possible reason can be the dependence of the compensation time constant on the spatial frequecy, which is small for high concentration of free ions. A second reason is the difference in modulation depth in these two techniques. The sine-Gordon equation, which had been developed for the description of the propagation of wave packages, was applied for the photorefractive wave mixing and a soliton solution was derived. For the first time, we observed experimentally the non-uniform distribution of the grating amplitude and the control of its profile by means of changes of input intensity ratio.

Investigation of X-ray storage phosphors. — Photoluminescence, photostimulated luminescence and EPR studies were carried out in Ce^{3+} doped $BaBr_2$ single crystals. Similar orthorombic $BaBr_2$ phases are present as nanocrystalline inclusions in appropriately prepared fluorobromozirconate glass ceramics and are expected to play a crucial role in the X-ray imaging applications of these ceramics.

History of science. — The chronology of the main events of the Gyulai -Tarján scientific school in the crystal physics from the fifties of the last century was collected and summarized on the basis of private notes. The scientific carriers of Prof. Gy. Turchányi and Dr. Z. Morlin belonging to this school were studied.

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Grants and international cooperations

OTKA T 037669	Geometrical, vibrational and electronic structure of borate crystals and their defects. (A. Watterich, 2002-2005)
OTKA T 026088	Fundamental processes of hologram fixing in photorefractive crystals. (L. Kovács, 1998-2002)
OTKA T 034262	Investigation and optimization of crystalline and glassy systems for data processing (G. Corradi, 2001-2004)
OTKA T 035044	Gyulai-Tarján school in crystal physics (E. Hartmann, 2001-2004).

HAS – Bulgarian Academy of Sciences joint project (No. 36): Growth and characterization of oxide crystals for optical application (L. Kovács, 2000-2003)

HAS – CNR (Italy) joint project (No. 4): Growth and complex characterization of rare-earth doped crystals for photonics (L. Kovács, 2001-2003)

HAS-Polish Academy of Sciences joint project: Structure of real crystals (A. Watterich, 2002-2004)

HAS – Polish Academy of Sciences joint project (No. 13): Investigation of structural defects in laser crystals (L. Kovács, 2002-2004)

TéT Austrian-Hungarian Intergovernmental S&T Project, A8/2001: Minerals and synthetic crystals for optical applications (L. Kovács, 2002-2003)

TéT German-Hungarian Intergovernmental S&T Project, D 11/01 Composition-dependent properties of oxide crystals for holographic applications (G. Corradi, 2002-2003)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP12: Growth and complex study of optical crystals (J. Janszky)

Long term visitor:

— dr. hab. L. Grigorjeva, Institute for Solid State Physics, University of Latvia, Riga, Latvia, 20 November 2002-11 December 2002, (Host: A. Watterich)

Publications

Articles

S.1. Millers D*, Grigorjeva L*, Pankratov V*, Chernov S*, Watterich A; Time-resolved spectroscopy of $ZnWO_4$; *Rad.Eff. Def. Solids*; **155,** 317-321, (2001)

S.2. Baraldi A*, Capelletti R*, Kovács L, Mora C*; FTIR spectroscopy of OH-induced defects in KTP single crystals; *Rad. Eff. Def. Solids;* **155,** 355-359, (2001)

S.3. Lengyel K, Kovács L, Mandula G, Rupp R*; Kinetics of OH^- ions in nearly stoichiometric $LiNbO_3$ crystals; *Ferroelectrics;* **257**, 255-262, (2001)

S.4. Corradi G, Lingner Th*, Kutsenko AB*, Dierolf V*, Polgár K, Spaeth JM*, von der Osten W*; Magneto-optical studies of Er^{3+} in $LiNbO_3$; *Rad. Eff. Def. Solids;* **155**, 223-227, (2001)

S.5. Williams RT*, Ucer KB*, Yochum HM*, Grigorjeva L*, Millers D*, Corradi G; Self-trapped electron and transient defect absorption in niobate and tungstate crystals; *Rad. Eff. Def. Solids;* **155**, 265-276, (2001)

S.6. Grigorjeva L*, Pankratov V*, Millers D*, Corradi G, Polgár K; Relaxation of electronic excitations in $LiNbO_3$ crystals; *Ferroelectrics;* **257,** 281-292, (2001)

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S.8. Watterich A, Kappers LA*, Gilliam OR*, Bartram RH*, Földvári I, Korecz L*; Paramagnetic and Diamagnetic Defects in e^- and UV-irradiated TeO_2.; *Nucl. Instr. and Meth. in Phys. Res.* B; **191/1-4**, 261-265, (2002)

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S.10. Kappers LA*, Gilliam OR*, Bartram RH *, Watterich A, Földvári I; Discovery of a self-trapped charge center in α-TeO_2; *Rad. Eff. Def. Solids*; accepted for publication.

S.11. Erdei S*, Schlecht RG*, Kovács L; Growth of PZN crystals with improved optical quality using the BSFT technique; *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control;* accepted for publication.

S.12. Kovács L, Lengyel K, Baraldi A*, Capelletti R*, Berkowski M*, Ryba-Romanowski W*; Hydroxyl ion absorption in $LaGaO_3$ single crystals; *J. Phys. and Chem. of Solids;* accepted for publication

S.13. Kovács L, Lengyel K, Péter Á, Polgár K, Beran A*; IR absorption spectroscopy of water in $CsLiB_6O_{10}$ crystals; *Optical Materials;* accepted for publication.

S.14. Capelletti R*, Beneventi P*, Kovács L, Fowler WB*; Multi-mode transitions of the tetrahedral MeO_4 units in sillenite single crystals; *Physical Review B;* accepted for publication.

S.15. Lengyel K, Kovács L, Baraldi A*, Capelletti R*, Berkowski M*, Ryba-Romanowski W*; The stretching vibration of hydroxyl ions in $LaGaO_3$; *Rad. Eff. Def. Solids;* accepted for publication

S.16 Mandula G, Ellabban MA*, Rupp RA*, Fally M*, Hartmann E, Kovács L, Polgár K; Activation energy of proton migration in Mn- and Fe-doped lithium niobate obtained by holographic methods; *Rad. Eff. Def. Solids;* accepted for publication.

S.17. Bugaychuk S*, Kovács L, Mandula G, Polgár K, Rupp RA*; Wave-mixing solitons in ferroelectric crystals; *Rad. Eff. Def. Solids;* accepted for publication.

Conference proceedings

S.18. Ellabban MA*, Mandula G, Rupp RA*, Fally M*, Hartmann E, Kovács L, Polgár K; Activation energy of thermal fixing in $LiNbO_3$: a comparative study; In: *Selected papers from Fifth International Conference on Correlation Optics, Chemistry, Ukraine, May 2001, Proc. of SPIE;* **4607**, 313-321, (2002)

S. 19. Ignatovych M*, Holovey V*, Watterich A, Vidóczy T*, Baranyai P*, Kelemen A*, Ogenko V*; Photoluminescence and radioluminescence study on Cu and Eu doped lithium tetraborates. In: *Proc. XIXth IUPAC Symposium on Photochemistry, Budapest, 2002*; pp 262-263, (2002).

S.20. Hartmann E, Péter Á, Lengyel K, Kovács L; Effect of the melt composition on the electrical conductivity and IR absorption of $CsLiB_6O_{10}$ crystals; In: *Proc. International Conference on Solid State Crystals, Zakopane, Poland, 14-18 Oct. 2002*; accepted for publication

Others

S.21. Hartmann E; Morlin Zoltán (1913-2002) (in Hungarian); *Fizikai Szemle;* **52,** 64, (2002)

See also R.1., R.3., R.11., T.12.

T. NONLINEAR AND QUANTUM OPTICS

P. Ádám, P. Domokos, A. Gábris[#], J. Janszky, A. Kárpáti[#], Zs. Kis, T. Kiss, Z. Kurucz[#], M. Koniorczyk[#], V. Szalay

Quantum interference. — Stochastic perturbation of two-level atoms strongly driven by a coherent light field is analyzed by the quantum-trajectory method. A method is developed for calculating the resonance fluorescence spectra from numerical simulations. It is shown that in the case of dominant incoherent perturbation, the stochastic noise can unexpectedly create phase correlation between the neighboring atomic dressed states. This phase correlation is responsible for quantum interference between the related transitions resulting in anomalous modifications of the resonance fluorescence spectra.

Quantum information, entanglement and teleportation. — Effects of noise and losses in the continuous variable teleportation scheme has been extensively studied. We have also analyzed the entanglement properties of certain two-mode generalizations of the usual optical Schrödinger cat state. These states were found to be appropriate for teleportation, hence opening ways to quantum communication based on coherent states. The teleportation schemes developed include perfect and imperfect teleportation of superpositions of $|0\rangle$, $|1\rangle$, $|2\rangle$ Fock states, and teleportation of states consisting of coherent states $|\pm\alpha\rangle$, $|\pm\alpha^*\rangle$.

Nuclear motions in molecules: dynamics and spectroscopy. — Reserarch papers and textbooks addressing the problem of internal rotation in a molecule explain symmetry properties of the torsional potential by local geometrical symmetries of the molecule. We have shown that symmetry properties of a torsional potential are consequences of both permutation inversion symmetry and a peculiar nature of torsional dynamics but have no relation to actual geometrical symmetries. To confirm the validity of our symmetry analysis a minimum energy torsional potential curve has been determined ab initio for acetaldehyde resulting in exact $2\pi/3$ periodicity, that no previous ab initio calculations achieved.

Application of adiabatic processes for coherent control. — We have continued the study of adiabatic population transfer processes with emphases on their application in different coherent control schemes. We have worked out a method to rotate single atomic qubits by means of the stimulated Raman adiabatic passage (STIRAP) process. We have shown that a light pulse propagating in a suitably prepared phaseonium medium can be converted with unity efficiency to another light pulse. This method provides an alternative way to frequency conversion in nonlinear crystals for weak fields.

Cavity quantum electrodynamics and laser cooling. — We study the cavity-induced light forces and cooling mechanisms on coherently driven neutral particles. We found various effects that rely on the indirect, cavity-mediated atom-atom interaction. In the case of N atoms simulatenously present in the cavity, the ensemble self-organizes to produce a maximized, collective scattering into the cavity. The self-created field leads then to a stable optical trapping of the many-atom system, the binding energy is being dissipated by a superfluorescent radiation into the cavity, and then via the cavity loss channel.

Quantum optics of microstructures. — We study the scattering of the radiation on neutral, polarizable particles situated in microstructures. Due to the tiny cross section of the incoming light field the scattering takes place in an unusual “strong coupling” limit.

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Grants and international cooperations

OTKA F 032341 Light-matter interaction in complex quantum systems (P. Domokos, 2000–2002)

OTKA T 034484 Application of nonclassical light in fundamental physical problems and in optical measurement methods (J. Janszky, 2001–2003)

OTKA F 032346 State reconstruction and preparation in quantum-optical systems (T. Kiss, 2000–2002)

OTKA T 034327 Reconstruction of vibrational potential energy surfaces of molecules, (V. Szalay, 2001–2003)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP12: Growth and complex study of optical crystals (J. Janszky and I. Földvári, 2000–2003)

TéT, Hungarian-Spanish Bilateral Intergovernmental S&T Cooperation E-10/2001: Calculation of the rotation-torsion spectrum of molecules with asymmetric top and asymmetric frame, and analysis of overlapping spectral bands by filter diagonalization (V. Szalay, 2001–2003)

Long term visitors

— Géza Tóth, Max Plank Institut für Quantenoptik, München, Germany, October-December, 2002 (host: J. Janszky)

Publications

Articles

T.1. Domokos P, Salzburger* T, Ritsch* H; Dissipative motion of an atom with transverse coherent driving in a cavity with many degenerate modes; *Physical Review A;* **66**, 043406/1-10, (2002)

T.2. Domokos P, Horak* P, Ritsch* H; Quantum description of light-pulse scattering on a single atom in waveguides; *Physical Review A;* **65**, 033832/1-12, (2002)

T.3. Farkas* Sz, Kurucz Z, Weiner* M; Poincare covariance of relativistic quantum position; *International Journal of Theoretical Physics;* **41**, 79-88 (2002)

T.4. Janszky J, Gábris A, Koniorczyk M, Vukics A, Asboth J; One-complex-plane representation: a coherent-state description of entanglement and teleportation; *Journal of Optics B: Quantum and Semiclassical Optics;* **4**, S213-S217, (2002)

T.5. Kárpáti A, Ádám P, Gawlik* W, Łobodziński* B, Janszky J; Quantum-trajectory approach to stochastically induced quantum-interference effects in coherently driven two-level atoms; *Physical Review A;* **66**, 023821/1-9, (2002)

T.6. Kis Z, Renzoni* F; Qubit rotation by stimulated Raman adiabatic passage; *Physical Review A;* **65,** 032318/1-4, (2002)

T.7. Kis Z, Stenholm* S; Optimal control approach for a degenerate STIRAP; *Journal of Modern Optics;* **49**, 111-124, (2002)

T.8. Paspalakis* E, Kis Z; Enhanced nonlinear generation in a three-level medium with spatially dependent coherence; *Optics Letters;* **27**, 1836-1838, (2002)

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T.10. Salzburger* T, Domokos P, Ritsch* H; Enhanced atom capturing in a high-Q cavity by help of several transverse modes; *Optics Express;* **10**, 1204-1214, (2002)

T.11. Szalay V, Császár* A G, Senent* M L; Symmetry analysis of internal rotation; *Journal of Chemical Physics;* **117**, 6489-6492, (2002),

T.12. Szalay V, Kovács L, Wöhlecke* M, Libowitzky* E; Stretching potential and equilibrium length of the OH bond in solids; *Chemical Physics Letters;* **354**, 56-61, (2002)

T.13. Vukics* A, Janszky J, Kobayashi* T; Nonideal teleportation in coherent-state basis; *Physical Review A;* **66**, 023809/1-9, (2002)

T.14. Domokos P, Ritsch* H; Collective cooling and self-organization of atoms in a cavity; *Physical Review Letters*; accepted for publication

T.15. Horak* P, Domokos P, Ritsch* H; Giant Lamb shift of atoms near lossy multimode optical micro-waveguides; *Europhysics Letters;* accepted for publication

T.16. Janszky J, Asbóth* J, Gábris A, Vukics* A, Koniorczyk M, Kobayashi* T; Two-mode Schrödinger cats, entanglement and teleportation; *Progress of Physics;* accepted for publication.

T.17. Kárpáti A, Ádám P, Gawlik* W, Łobodziński* B, Janszky J; Quantum-trajectory approach to stochastically-induced quantum interference; *Progress of Physics;* accepted for publication

Conference proceedings

T.18. Gangl* M, Horak* P, Domokos P, Ritsch* H; Collective cooling of neutral particles in cavities without spontaneous emission; In: *Proceedings of the Symposium on Modern Problems of Laser Physics (MPLP 2000)*, Akademgorodok Novosibirsk, Russia, Eds.: S. I. Bagayev and V. I. Denisov; pp 257-268, (2001)

T.19. Kiss T, Domokos P, Janszky J; State selective manipulation of molecules: implementing Maxwell's demon; In: *AIP Conference Proceedings;* **643,** 259-266, (2002)

T.20. Koniorczyk M, Janszky J; Photon number conservation and photon interference; In: *First International Workshop on Classical and Quantum Interference, 25-26 October, 2001, Olomouc, Czech Republic*, Eds.: Jan Peřina, Miroslav Hrabovský, and Jaromir Křepelka, Proceedings of SPIE; **4888**, pp 1-8, (2002); invited paper

T.21. Ritsch[*]H, Domokos P, Horak[*]P, Gangl[*] M; Optical cooling in high-Q multimode cavities; In: *Proc. of the XV International Conference on Laser Spectroscopy (ICOLS 2001),* Ed:V. Vuletic, S. Chu, A. J. Kerman, and Cheng Chin, Word Scientific; pp 184-192, (2002)

T.22. Domokos P, Horak[*] P, Ritsch[*] H; Quantum theory of dipole scattering of photons in micro-waveguides; In: *Proc. of the Wigner Centennial Conference, 8-12 July, 2002, Pécs, Hungary;* accepted for publication

T.23. Gawlik[*] W, Łobodziński[*] B, Ádám P, Kárpáti A, Janszky J; Stochastically induced quantum interference incoherently driven two-level system; In: *Proc. of the Wigner Centennial Conference, 8-12 July, 2002, Pécs, Hungary;* accepted for publication

T.24. Janszky J, Asbóth J, Gábris A, Vukics A, Koniorczyk M, Kobayashi[*] T; Two-mode Scrödinger cats: entanglement and teleportation; In: *Proc. of the Wigner Centennial Conference, 8-12 July, 2002, Pécs, Hungary;* accepted for publication

T.25. Kárpáti A and Kis Z; Adiabatic population transfer in a multi-level Λ system; In: *Proc. of the Wigner Centennial Conference, 8-12 July, 2002, Pécs, Hungary;* accepted for publication

T.26. Kis Z, Paspalakis[*] E, Renzoni[*] F, Stenholm[*] S; Controlling material by light and light my material via adiabatic processes; In: *Proc. of the Wigner Centennial Conference, 8-12 July, 2002, Pécs, Hungary;* accepted for publication

T.27. Kiss T, Ádám P, Janszky J; Gauss filtered back projection for the reconstruction of the Wigner function; In: *Proc. of the Wigner Centennial Conference, 8-12 July, 2002, Pécs, Hungary;* accepted for publication

T.28. Koniorczyk M, Bužek[*] V; Simulation of Wigner-Weisskopf decay on simple quantum circuits: a case study; In: *Proc. of the Wigner Centennial Conference, 8-12 July, 2002, Pécs, Hungary;* accepted for publication

T.29. Vukics A, Janszky J, and Kobayashi[*] T; Nonideal teleportation in coherent-state basis; in: *Proc. of the Wigner Centennial Conference, 8-12 July, 2002, Pécs, Hungary;* accepted for publication

See also O.1.

THE SZFKI AS THE HOST INSTITUTE OF THE CENTRE OF EXCELLENCE "KFKI-CMRC"

Our institute, together with the KFKI Atomic Energy Research Institute, the KFKI Research Institute for Particle and Nuclear Physics and the Research Institute for Technical Physics and Material Science established an organisation, the KFKI Condensed Matter Research Center (KFKI-CMRC) in order to coordinate the research activity in the field of condensed matter physics and applications at the KFKI campus. In 2000 the KFKI-CMRC became a **"Centre of Excellence"** within the 5th Framework programme of the European Union.

"Centres of Excellence" is part of a programme launched by the European Commission in order to contribute to the restructuring of the science and technology sector of the newly associated states. As many as 34 excellent research centres have been selected in these countries and are supported to improve their links with other European centres through different types of activities, such as invitation of experienced scientists, training of Ph.D. students and post-doctoral researchers, organising workshops and conferences, etc.

Our project started on the 1st of November 2000 and will terminate on the 31st of October 2003, right now we have surpassed half time. The projects coordinated by scientists of the Research Institute for Solid State Physics and Optics are the following:

- WP1 Enhancing regional users' access to the new Cold Neutron Facility at the Budapest Research Reactor (Dr. L. Rosta)
- WP7 Condensed matter theory (Pr. F. Iglói)
- WP8 Atomic level structural studies by photons and neutrons (Dr. Gy. Faigel)
- WP9 Nation-wide Co-operation for the Study of Non-equilibrium Metallic Materials (Dr. T. Kemény)
- WP11 Interaction of light with condensed matter (Dr. N. Éber)
- WP12 Growth and complex study of optical crystals (Pr. J. Janszky)

In the current reporting period the implementation of the project goals has continued successfully. As a result 18 scientific papers have been published in international journals and 15 lectures have been given at international conferences. So far since the beginning of the project we have employed 28 foreign scientists from 10 different countries as long term visitors for 146 months altogether, 62 foreign scientists visited our centre for a short period of time. We have organised 17 international conferences, workshops and have purchased durable equipment for 23179 Euro. In June 2002 the second yearly meeting of the Centres of Excellence took place in Budapest. It proved to be an excellent opportunity to analyse the results and discuss the possibilities of stronger co-operation among the existing centres. As a result of the meeting several Expression of Interests were submitted. Intensive work began to join different networks that are now forming to be part of the 6th Framework Programme.

In November 2002 the 6th Framework Programme has been launched in Brussels. Several modifications have been made compared to the previous Framework Programme; our managers and scientists are continuously studying these changes in order to ensure successful participation.

EDUCATION

Graduate and postgraduate courses, 2002

— Electrodynamics of continuous media (F. Woynarovich, ELTE[2])
— Completely integrable many body systems (F. Woynarovich, ELTE)
— Solid state physics (J. Sólyom, ELTE)
— Advanced solid state physics I-II (J. Sólyom, ELTE)
— Statistical physics (F. Iglói, SZTE[3])
— Applications in statistical physics (F. Iglói, SZTE)
— Magnetism I. (P. Fazekas, BME[4])
— Magnetism II. (P. Fazekas, BME)
— Advanced solid state physics III. (I. Tüttő, ELTE)
— Optical properties of solid state (I. Tüttő, ELTE)
— Electronic states in solids (J. Kollár, ELTE)
— Metal physics (J. Kollár, BME-ELTE)
— Solid state research I-II (I. Vincze, ELTE)
— Amorphous and crystalline materials (P. Deák*, S. Kugler* and T. Kemény, BME)
— Modern theory of nucleation (L. Gránásy, ELTE)
— Macromolecules (S. Pekker, ELTE)
— Spectroscopy and materials structure (K. Kamarás, BME)
— Methods in materials science (K. Kamarás, BME)
— Infrared and Raman spectroscopy (K. Kamarás, BME)
— Physics of liquid crystals and polymers (Á. Buka, N. Éber, ELTE)
— Pattern formation in complex systems (Á. Buka, ELTE)
— Liquid crystals, their chemistry and chemical physics (K. Fodor-Csorba, ELTE)
— Advanced material technology (G. Konczos, BME and ELTE)
— NMR spectroscopy (K. Tompa, BME)
— Group theory in solid state research (G. Kriza, BME)
— Superconductivity (G. Kriza, BME)
— Neutron scattering in condensed matter (L. Cser, ELTE)
— Disorder in condensed phases (L. Pusztai, ELTE)

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

— Neutrons in condensed matter research (L. Pusztai, BME)

— Optical methods in experimental solid state physics (Z. Szentirmay, ELTE).

— Physics of amorphous matter I. (M. Koós and I. Pócsik, SZTE)

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

— Crystal physics of optical crystals (I. Földvári, Á. Péter, BME)

— Growth, orientation and processing of nonlinear optical crystals (in: Applied Lasertechnics, I. Földvári, Á. Péter, BME)

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

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

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

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

— Statistical quantum optics (J. Janszky ELTE)

— Quantum Optics (J. Janszky, PTE[5])

— Quantum mechanics I. (P. Ádám, PTE)

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

— Vector calculus I (A. Gábris, PTE)

— Vector calculus II (A. Kárpáti, PTE)

— Vector calculus III (Z. Kurucz, PTE)

Laboratory practice and seminars

— Solid State Physics seminar (J. Sólyom, ELTE)

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

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

— Basic experimental physics (L. Gránásy, BME)

— Atomic and molecular physics laboratory (K. Kamarás, ELTE)

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

— NMR spectroscopy (K. Tompa, ELTE and BME)

— Physical Chemistry Laboratory Practice (L. Péter, ELTE)

— Advanced solid state physics laboratory (P. Matus and L. Németh, ELTE and BME)

— Neutron scattering (L. Rosta, BME)

— Neutron scattering and hands-on-training at BRR (L. Cser, Gy. Török, E. Rétfalvi, BME)

[5] PTE = University of Pécs

— Neutron scattering in materials research (L. Rosta, ME[6])

— Computing in chemistry (L. Pusztai, ELTE)

— Gamma-dosimeter calibration (Z. Somogyvári, BME)

— Neutron diffractometer acquisition- and control software (E. Sváb, BME)

— Medical application of lasers (Z. Gy. Horváth, Medical Laser Center)

— Electrodynamics (K. Lengyel, PTE)

— Introduction to physics (K. Lengyel, PTE)

— Calculus and linear algebra problem solving seminar (M. Koniorczyk, PTE)

— Computer aided evaluation of measurement data (M. Koniorczyk, PTE)

— Physics seminar (P. Ádám, PTE)

— Quantum mechanics I. (A. Gábris, PTE)

Diploma works

— B. Almási (ELTE): Study of hydrogen diffusion in Pd_XAg_{100-X} alloys by electrochemical methods (Consultant: L. Péter)

— Z. Kupay (ELTE): Electrochemical preparation and study of Co-Cu-Me/Cu multilayers (Consultant: L. Péter)

— Á. Pallinger (ELTE): Study of current distribution in high-T_c superconductors (Consultant: B. Sas)

— Á. Bányász (ELTE): Process controll and data acquisition software developed for femtosecond time resolved spectroscopic measuerements on chemical samples (Consultant: R. Szipőcs)

— B. Rózsa (ELTE): Two photon microscopy (Consultant: R. Szipőcs)

Ph. D. students

F. Borondics (ELTE): Investigation of fulleride salts by Raman spectroscopy. (Supervisor: G. Oszlányi)

Z. Jurek (BME): Atom resolution imaging of non-periodic systems. (Supervisor: G. Faigel)

G. Klupp (ELTE): Investigation of alkali fulleride salts by infrared spectroscopy (Supervisor: K. Kamarás)

É. Kováts (ELTE): Addition reaction of fullerenes and related compounds in solid phase (Supervisor: S. Pekker)

Sz. Németh (BME): Instabilities and convective patterns in liquid crystals. (Supervisor: Á. Buka)

[6] ME = University of Miskolc

H. Nádasi (ELTE): Banana shaped liquid crystals and their physico-chemical properties. (Supervisor: K. Fodor-Csorba)

A. Bárdos (BME): Preparation, characterization and application of Fe-based bulk amorphous alloys (Co-supervisor: L.K. Varga)

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

Zs. Gercsi (ELTE – ENS de Cachan, France): Tayloring the hysteresis loop for high frequency and high temperature applications of nanocrystalline alloys (Hungarian co-supervisor: L.K. Varga)

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

A. Kákay (ELTE): Magnetic nanocomposites: modelling and experiments (Supervisor: L.K. Varga)

P. Matus (BME): NMR study of metals with correlated electronic system (Supervisor: G. Kriza)

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

I. Pethes (BME): Experiments on moving glasses (Supervisor: G. Kriza)

I. Varga (BME): Magnetic domain contrast studies and image processing by SEM (Supervisor: L. Pogány)

L. Almásy (ELTE): Investigation of liquid mixtures by neutron scattering (Supervisor: L. Cser)

A. Len (ELTE): Small angle neutron scattering study of sintered materials (Supervisor: L. Rosta)

E. Rétfalvi (BME): Irradiation damage study of materials of technological importance by neutron scattering technique (Supervisor: L. Rosta)

Zs. Sánta (ELTE): Materials structures by time-of-flight neutron diffraction (Supervisor: L. Rosta)

G. Vaspál (ELTE): Applied Neutron Optics (Supervisor: L. Cser)

Z. Somogyvári (BME): Magnetic and atomic structure investigations by neutron diffraction (Supervisor: E. Sváb)

I. Harsányi (ELTE): The structure of aqueous electrolyte solutions (Supervisor: L. Pusztai)

M. Veres (BME): Physical properties of graphitic carbon nano-structures (Supervisor: I. Pócsik)

M. Füle (SzTE): Optical absorption investigation of hydrogenated amorphous carbon films (Supervisor: M. Koós)

S. Tóth (SzTE): Optical absorption investigation of hydrogenated amorphous carbon films (Supervisor: M. Koós)

D. Oszetzky (BME): Investigation of squeezed light (Supervisor: A. Czitrovszky)

Z. Lipp (BME): Photon correlation measurements (Supervisor: P. Jani)

H. Moussambi (Université de Metz): Growth of beta-BBO single crystals by direct Czochralski method (Hungarian co-supervisor: K. Polgár)

T. Ujvári (BME): High capacity and fidelity holographic reorders specified by multiplexing and security measures (Co-supervisor: I. Földvári)

K. Lengyel (PTE): Study of OH^- ion absorption in non-linear optical crystals (Supervisor: L. Kovács)

A. Gábris (SZTE): Nonlinear photonic crystals and quantum optical processes therein (Supervisor: J. Janszky)

A. Kárpáti (PTE): Quantum phenomena in photonic band-gap structures (Supervisor: P. Ádám)

M. Koniorczyk (PTE): Nonlocality in quantum optical systems (Supervisor: J. Janszky)

Z. Kurucz (SZTE): Quantum state manipulations and quantum information theory (Supervisor: J. Janszky)

Dissertations

E. Mátyus: Mesomorphism of new type banana shaped liquid crystals. (Ph.D., ELTE)

P. Kamasa: Method of sensitivity enhancement in deuterium muclear magnetic resonance spectroscopy by digital phase-sensitivity detection (Ph.D., University of Debrecen)

G. Lasanda: Proton magnetic resonance spectrum and second moment in amorphous Zr-Ni-Cu-H alloys (Ph.D., ELTE)

L. Almásy: Structure and Dynamics in Binary Mixtures with Limited Miscibility (Ph.D., ELTE/Univ. Marie et Pierre Curie, Paris)

S. Lakó: Femtosecond nonlinear optics (Ph.D., SZTE, Szeged)

K. Szőcs: Photosensitisation of *Escherichia coli B.* bacteria by endogenous porphyrin derivatives (Ph.D., SE, Budapest)

G. Corradi: Dopant ions and radiation point defects in non-linear optical oxide crystals (D. Sc., Hungarian Academy of Sciences).

L. Kovács: Vibrational modes of hydroxyl ions and oxygen terahedra in oxide crystals (D.Sc., Hungarian Academy of Sciences).

AWARDS

— F. Woynarovich, Széchenyi Professorship (2000-2003)

— G. Fáth, Bolyai Grant (1999-2002)

— G. Fáth, Jánossy Prize of the Loránd Eötvös Physical Society, 2002

— Ö. Legeza, Bolyai Grant (2000-2003)

— K. Penc, Bolyai Grant (1999-2002)

— K. Penc, OTKA post-doctoral grant D 32689

— J. Sólyom, Széchenyi Professorship (1999-2002)

— J. Kollár, Széchenyi Professorship (2000-2003)

— F. Woynarovich, Széchenyi Professorship (2000-2003)

— D. Kaptás, Bolyai grant (1999-2002)

— L. Gránásy, Széchenyi Professorship (1999-2003)

— K. Kamarás, Széchenyi Professorship (1998-2002)

— G. Kriza, Széchenyi Professorship (1999-2002)

— M. Bokor, Bolyai Grant (2001-2004)

— K. Tompa, Main Physics Award of HAS (2001)

— L. Cser, GENIUS Grand Prize, at the IV. GENIUS Inventor's International Exhibition, Budapest, 2002

— J. Füzi, Diploma of Merit of Bolyai Research Fellowship, 2002.

— L. Pusztai, Széchenyi Professorship (2000-2003)

— L. Csillag, Diploma of Merit of the Secretary General, H.A.S. (2002)

— R. Szipőcs, Bolyai Grant (1999-2002)

— I. Földvári, Széchenyi Professorship, (2000-2003)

— Z. Kis, Bolyai Grant (2001-2003)

— Z. Kis, Young Researcher Award of the Hungarian Academy of Sciences (2002)

— Z. Kis, Publication Award of SZFKI (2002)

CONFERENCES

— 2nd Int. Workshop on **Electrodeposited Nanostructures** (Budapest, Hungary, Oct. 11-12, 2002). Organizers: I. Bakonyi (chair), L. Péter (secretary), E. Tóth-Kádár and J. Tóth. 43 registered participants from 12 countries and a few informal visitors from the campus attended the meeting. In the 14 scientific lectures, the speakers presented a state-of-the-art picture on the application of electrochemical deposition for preparation of nanostructures. Special attention was paid to the pulse plating techniques, template deposition of multilayers and nanowires, magnetism and magnetotransport in multilayers and structure of electrodeposited amorphous and layered materials. One technical presentation was held about an ongoing work to promote the co-operation between European scientists who deal with pulse plating. The oral presentations were followed by a poster session where 10 posters were presented. As a special part of the workshop, the organizers presented their laboratories and scientific instruments to the participants. The closing session of the workshop gave the opportunity for an open scientific discussion. The approximate time and the most likely venue of the next workshop were also selected.

— A training school **"Central European Course and Hands-on-Training on Neutron Scattering"** was organised at the Budapest Research Reactor between December 7-12, 2001. Organiser: L. Rosta. The course consisted of 4 days lectures given by renowned European scientists and experimental works on several neutron spectrometers. The course provided both valuable scientific and practical information on neutron scattering techniques and introduced the participants (34 people from 8 countries) – current and potential users, most of them coming from Central European countries – to the possibilities offered by the facilities of Budapest Neutron Centre, the most important large scale facilities in the region.

— The 17th Committee meeting of the **European Neutron Scattering Association and European Neutron Round Table** was held in Budapest, October 24-25, 2002. Organisers: L. Rosta, J. Füzi. The 42 delegates of the national neutron research organisations and leading scientists of the major European neutron centres, being present at this meeting, represent the nearly 5000 researches working in this field. This ENSA/NRT body meets regularly every half-year and deals essentially with strategic problems and co-ordination of this interdisciplinary research activity. The major issue of the current meeting was the preparation of neutron research proposals, integrated initiatives for the EU 6th Framework Programme.

— **Wigner Centennial Conference,** Pécs, Hungary, 8-12 July, 2002. Organized jointly by the Department of Nonlinear and Quantum Optics of the Research Institute for Solid State Physics and Optics with the Physics Institute of University of Pécs (J. Janszky, chair, P. Ádám, secretary). Wigner Jenő Pál (Eugene Paul Wigner), one of the greatest Nobel prize laurate physicists of the 20th century was born in 1902. The physics community celebrated the Wigner Centennial year in various forms. With the contribution of 166 participants from 34 countries, the Centennial Conference in Commemoration of Eugene Paul Wigner intended to cover at least partly the present state of arts of the large variety of fields to which Wigner made important contributions, breaking new paths in many domains of physics. Proceedings will be published in Acta Physica Hungarica.

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