ANNUAL REPORT

2003

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 2003

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

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Dear Reader,

It is my pleasure to hand over the 10th edition of the Annual Report of the Research Institute for Solid State Physics and Optics in 2003.

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. In recent years financial contribution from the Hungarian Academy of Sciences increased due to the general salary growth issued by the government for all employees in this sector in 2002.

Our institute employs 170 people from which there are approximately 100 scientists. During recent years our employees' age categories have shifted. More and more young researchers join our institute, where our scientists have 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. This year we have published more than 230 papers in high quality international journals and conference proceedings. The number of these publications is similar to that of the previous years. In 2003 three of our scientists have become Doctors of the Hungarian Academy of Sciences (DSc). It is a tradition in our institute to hand out awards for publication and applied research. In 2003 awards were shared in both categories. The publication prize was given to Imre Bakonyi and Zoltán Donkó, the applied research prize was taken by Gergely Bánó and László Péter.

Since Hungary has joined the EU 6th 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) has taken part in the "*Centre of Excellence" programme of the European Union.* The program has been running for three years and will reach its conclusion in early next year. A description of the work conducted at the Centre during these three years can be found at the end of this annual report.

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 9% (EU funds in 2001 were 13%; in 2002 8% of our budget). 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.

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 http://www.szfki.hu

Budapest, 29 november, 2017

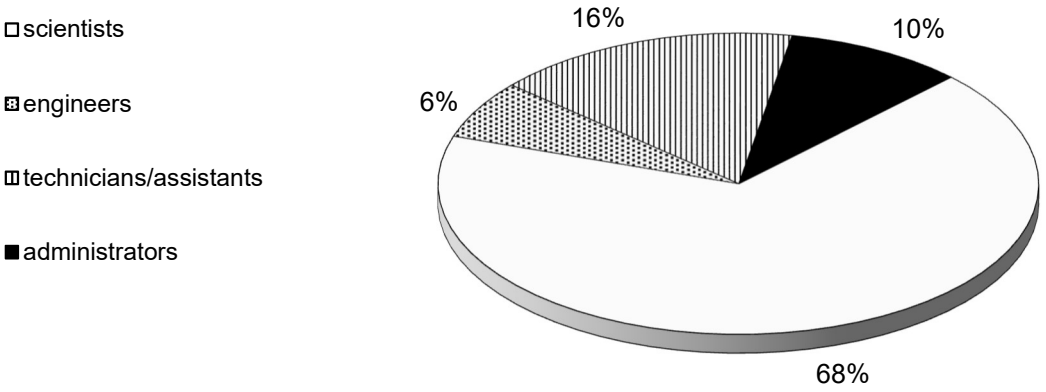
János Kollár

Director

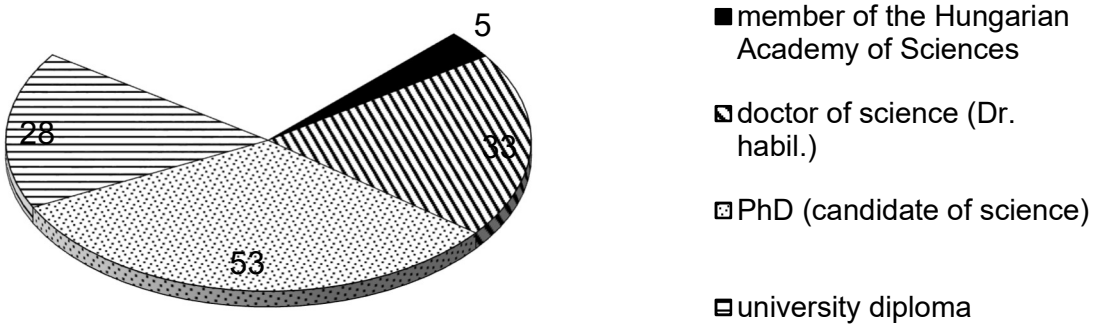
Key figures

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

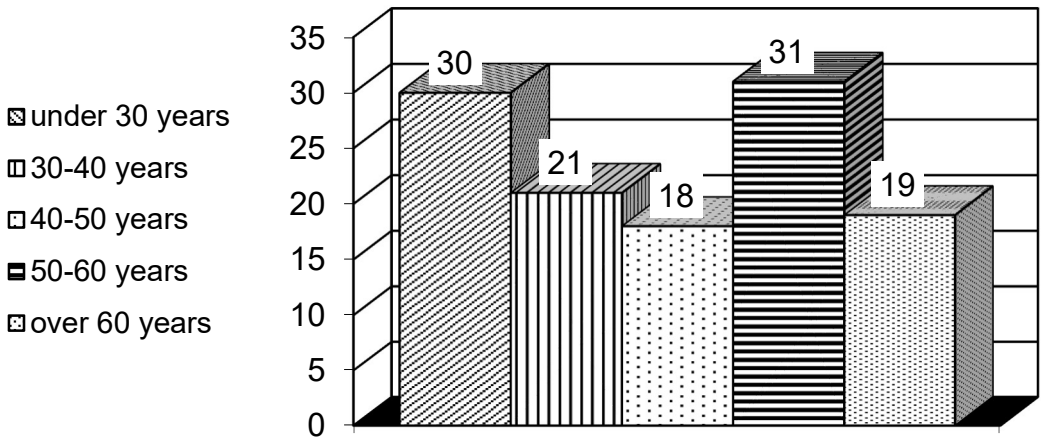
a) by professions:



b) by scientific titles/degrees:

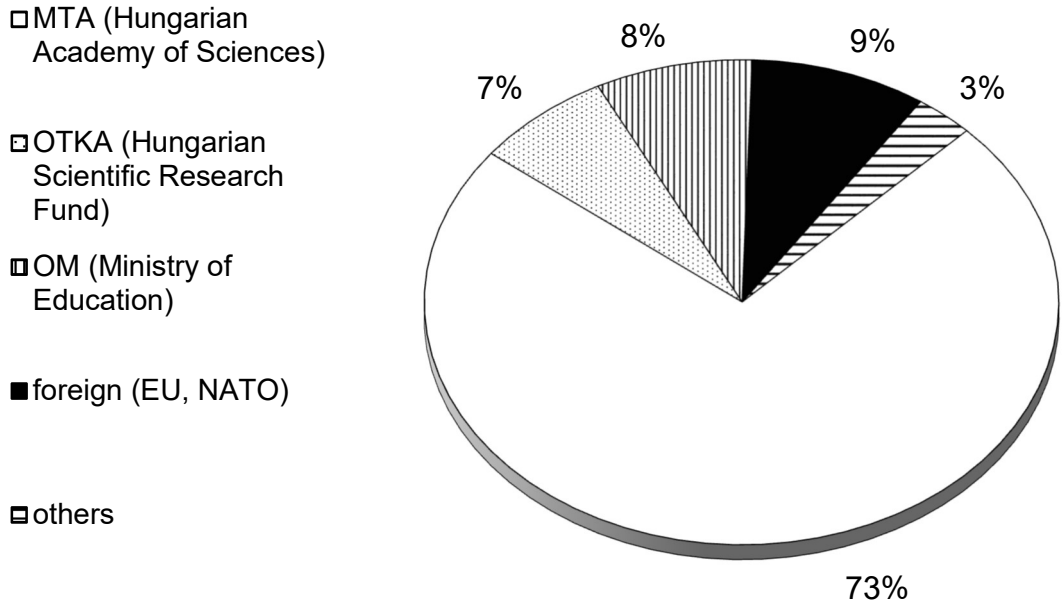


c) by ages:

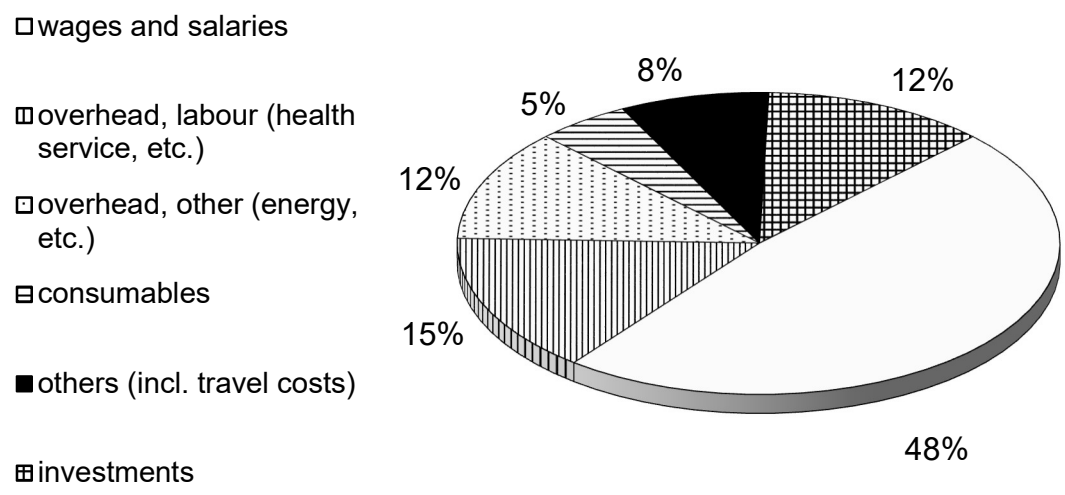


Financial management

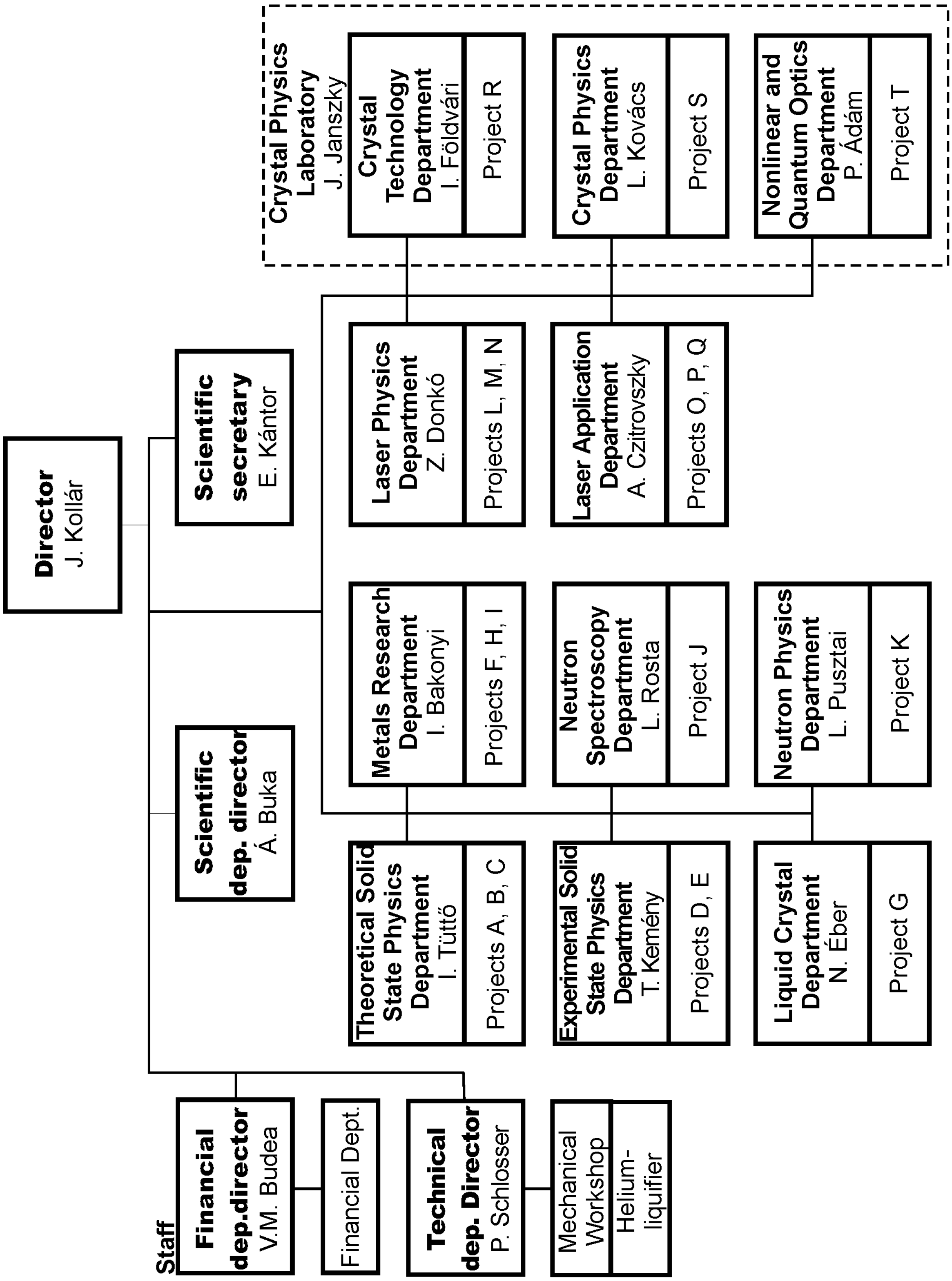
a) Sources of operation costs:



b) Distribution of expenditures:



Structure of the Research Institute for Solid State Physics and Optics



A. STRONGLY CORRELATED SYSTEMS

J. Sólyom, G. Fáth, Ö. Legeza, K. Penc, E. Szirmai[#], 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.

While fractional excitations are commonplace in the one-dimensional physics, they are much rarer in higher dimensions. We have shown that on the lattice made of corner shared tetrahedra (pyrochlore lattice) fractional excitations of charge 1/2 are supported in a Hubbard-model extended with nearest neighbour repulsion - an added electron will decompose into two, spatially separated, objects, with charge 1/2 each. It is made possible by the exponentially large degeneracy of the ground state at quarter filling, and is directly related to the ice-problem. We gave a topological classifications of the excitations, and numerically determined the bandwidth for a single added electron.

Fermionic models. — We continued the development and application of the momentum space and quantum chemistry versions of the density matrix renormalization group method (MS-DMRG and QC-DMRG, respectively). The main difference between MS-DMRG and the standard, real space version is that in the latter case each lattice site is equivalent and carries the same amount of information, while the k-points or molecular orbitals lying closer to or farther away from the Fermi surface have different information content. The number of states needed to achieve a prescribed accuracy and the convergence depends strongly on the ordering of the states. We have developed a dynamical block state selection (DBSS) procedure to improve the accuracy. In order to optimize the ordering we have studied the separability and entanglement of the target state for the 1-D Hubbard model and various molecules. A new initialization procedure has been developed which maximizes the Kullback-Leibler entropy and extends the active space (AS) in a dynamical fashion. The dynamically extended active space (DEAS) procedure reduces significantly the effective system size during the first half sweep and accelerates the speed of convergence of MS-DMRG and QC-DMRG. By analyzing the behaviour of von Neumann entropy we have found criteria that help to fasten convergence.

The effect of ordering has been related to the field of quantum data compression. We have applied the concepts of quantum information theory for the first time within the context of DMRG and have shown how DMRG can be interpreted from the point of view of synergetics as a dynamical system. Using this analogy we have studied the response to incident messages, the change of the relative importance of messages.

We developed a functional integral method to calculate the contributions of saddle point fluctuations to the free energy of Bethe Ansatz systems. These contributions give O(1) corrections to the macroscopic value. We analyzed the case of δ Bose gas in more detail.

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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.

We presented an exactly solvable example for localization due to ohmic heat bath in zero external field. The size of the ground state of a damped harmonic oscillator remains finite as the harmonic potential vanishes.

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Grants

OTKA[1] T 030173	Theoretical study of magnetically or electrically low-dimensional models (J. Sólyom, 1999-2003)
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 T 043330	Theoretical study of strongly correlated low-dimensional systems (J. Sólyom, 2003-2006)

Long term visitors

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

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

Publications

Articles

A.1. Fulde[*] P, Penc K, Shannon[*] N; Fractional charges in pyrochlore lattices; *Ann Phys; Berlin*, **11**, 892-900, 2002

A.2. Penc K, Mambrini[*] M, Fazekas P, Mila[*] F; Quantum phase transition in the SU(4) spin-orbital model on the triangular lattice; *Phys Rev B*; **68**, 012408/1-4, 2003

[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*; **68**, 134445/1-6, 2003

A.4. Legeza Ö, Röder* J, Hess* BA; QC-DMRG study of the ionic-neutral curve crossing of LiF; *Mol Phys*; **101**, 2019-2031, 2003

A.5. Fáth G, Sárváry* M; Adoption dynamics in buyer-side exchanges; *Quantitative Marketing and Economics*; **1**, 305-335, 2003

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*; **67,** 125114/1-10, 2003

A.7 Legeza Ö, Sólyom J; Optimizing the density-matrix renormalization group method using quantum information entropy; *Phys Rev B*; 68, 195116/1-19, 2003

Books

A.8. Sólyom J; A modern szilárdtestfizika alapjai, II kötet. Elektronok a szilárd testekben; (Fundamentals of solid state physics, Vol. II. Electrons in solids, in Hungarian); *ELTE Eötvös Kiadó*; 2003, 580 p

A.9. Sólyom J; A modern szilárdtestfizika alapjai, III kötet. Kölcsönhatás az elektronok között; (Fundamentals of solid state physics, Vol. III. Interaction between the electrons, in Hungarian); *ELTE Eötvös Kiadó*; 2003, 580 p

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. —The effect of quenched disorder on the low-energy and low-temperature properties of various two- and three-dimensional Heisenberg models is studied by a numerical strong disorder renormalization group method. For strong enough disorder we have identified two relevant fixed points, in which the gap exponent, ω, describing the low-energy tail of the gap distribution, $P(\Delta) \sim \Delta^{\omega}$ is independent of disorder, the strength of couplings and the value of the spin. The dynamical behavior of non-frustrated random antiferromagnetic models is controlled by a singlet-like fixed point, whereas for frustrated models the fixed point corresponds to a large spin formation and the gap exponent is given by $\omega \approx 0$. Another type of universality classes is observed at quantum critical points and in dimerized phases but no infinite randomness behavior is found, in contrast to one-dimensional models.

The effect of quenched disorder on non-equilibrium phase transitions in the directed percolation universality class is studied by a strong disorder renormalization group approach and by density matrix renormalization group calculations. We show that for sufficiently strong disorder the critical behavior is controlled by a strong disorder fixed point and in one dimension the critical exponents are conjectured to be exact: $\beta = (3-\sqrt{5})/2$ and $\nu_{\perp} = 2$. For disorder strengths outside the attractive region of this fixed point, disorder dependent critical exponents are detected. Existing numerical results in two dimensions can be interpreted within a similar scenario.

Scaling behaviour in a spin model with locally broken spin symmetry has been investigated carrying out large-scale simulations. The multispecies annihilating random walk transition found at zero branching rate was investigated now concerning the cluster scaling behavior of the underlying spins. Generic power law behaviors were found in the active phase as well as at the critical point with fulfillment of the hyperscaling law. It was found, however, that scaling laws connecting bulk and cluster exponents are broken at this transition.

We studied the appearance of normal and anomalous diffusion in a classical one-dimensional system consisting of an overdamped particle dragged by a constant external field and hindered by a quenched random sequence of scatterers. No time-dependent random force was taken into consideration. We computed the diffusion constant and found the transition between propagation and localization to be analogous to phase transitions.

Quantum systems. — The investigation of the dynamics of spin-1 Bose gases at and below the temperature of the Bose-Einstein condensation has been continued. We have shown that the Green's functions and the various correlation functions (describing collective excitations) are in harmony with the equation of state in the self-consistent Hartree-Fock approximation only if two types of Feynman diagrams are summed up to infinite order. The results are applied to gases of ^{23}Na and ^{87}Rb atoms in the density and spin channels.

In finite temperature field theory we have pointed out that universal properties show up near the threshold where a particle can decay and worked out these properties.

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Grants and international cooperations

OTKA T029552 Study of atomic systems (P. Szépfalusy, 1999-2003)
OTKA T042914 Mathematical study of interacting Fermi and Bose systems (A. Sütő, 2003-2005)
OTKA T034183 Disordered quantum spin systems (F. Iglói, 2001-2004)
OTKA T034784 Scaling behavior and universality in non-equilibrium systems (N. Menyhárd, 2001-2003)
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. Juhász R, Iglói F; Percolation in random environment; *Phys Rev E*; **66**, 056113/1-7, 2002

B.2. 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*; **66,** 117701/1-4, 2002

B.3. Hooyberghs* J, Iglói F, Vanderzande* C; Infinite randomness fixed point description of absorbing state phase transitions with quenched disorder; *Phys Rev Lett*; **90,** 100601/1-4, 2003.

B.4. Lin* Y-C, Mélin* R, Rieger* H, Iglói F; Low-energy fixed points of random Heisenberg models; *Phys Rev B*; **68**, 024424/1-10, 2003

B.5. Anglés d'Auriac* J-Ch, Iglói F; Phase transition in the 2d random Potts model in the large-q limit; *Phys Rev Lett*; **90**, 190601/1-4, 2003

B.6. Menyhárd N, Ódor* G; Multispecies annihilating random-walk transition at zero branching rate: Cluster scaling behavior in a spin model; *Phys Rev E*; **68,** 056106/1-6, 2003

B.7. Sütő A; WKB for quantum spins; *Physica A*; **321,** 493-497, 2003

B.8. Sütő A; Thermodynamic limit and proof of condensation for trapped bosons; *J Stat Phys*; **112,** 375-396, 2003

B.9. Kunz* H, Livi* R, Sütő A; Mechanical model of normal and anomalous diffusion; *Phys Rev E*; **67,** 011102, 2003

B.10. Szirmai* G, Szépfalusy P, Kis-Szabó* K; Energies and damping rates of elementary excitations in spin-1 Bose-Einstein condensed gases; *Phys Rev A*; **68**, 023612/1-19, 2003

B.11. Patkós* A, Szép* Zs, Szépfalusy P; Universal threshold enhancement; *Phys Rev D***; 68**, 047701/1-4, 2003

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 recently developed new method to calculate the total energy for random substitutional alloys has been applied for bulk metals and surfaces:

— **Alloy steel design** has always been facing a central problem: When designing for a specific property, a simultaneous significant improvement on other properties is very rarely achieved. For instance, it is difficult to design a material that combines high values of the two most important mechanical characteristics of solids, hardness and ductility. Using the most recent quantum theories of random alloys, in collaboration with Swedish researchers we addressed a similar problem in the design of *austenitic stainless steels*, namely, to combine high mechanical characteristics with good corrosion resistance. We have shown that an optimal combination of hardness, ductility, and corrosion resistance can be achieved in alloys within the compositional range of commercial *stainless steels*. We predicted that a) $Fe_{58}Cr_{18}Ni_{24}$ alloys possess an intermediate hardness combined with improved ductility and excellent corrosion resistance, and that b) Os and Ir alloying additions further improve the basic properties of this outstanding class of alloy steels.

— Using our ab initio method we have investigated the composition and properties of the boundary between the **Earth's metallic core** and its **silicate mantle**. We studied the interaction between Fe, which is the dominant component of the Earth's core, and silica (SiO_2). We showed that the chemical interaction drastically depend on pressure: at low pressure iron-oxide and FeSi alloys are formed, while at high pressure the FeSi alloys dissociate into pure Fe and CsCl structured FeSi compound. These results explain the anomalously high electric conductivity of core-mantle boundary.

— We have proposed a self-consistent method for electronic structure calculations of **correlated systems**, which combines the local spin-density approximation (LSDA) and the dynamical mean field theory (DMFT). The LSDA part is based on the EMTO approach, meanwhile the DMFT uses a perturbation scheme that includes the T-matrix with fluctuation exchange approximation. We present results on the electronic structure calculations for bulk 3d transition metals (Cr, Fe and Ni) and for Fe/Cr magnetic multilayers.

— Using the density functional theory, formulated within the framework of the EMTO-FCD, we have calculated the **surface stress** for the (111) free surfaces of the fcc non-magnetic transition metals. Good agreement is obtained with the available *ab initio* data for Pd, Ir and Au, while for Pt we predict a surface stress, which is about 33% lower compared to former theoretical results. The present surface stress values for the 4d and 5d fcc metals show the typical trend characteristic for the cohesive or surface energies of d series.

Motivated by the recent suggestion of **octupolar ordering** as primary order parameter in NpO_2 compounds, we studied f-electron lattice models which are capable of supporting octupolar, as well as dipolar and quadrupolar, order. Analyzing the properties of the Γ_8 ground-state quartet, we found that because of a peculiar single-ion anisotropy of this subspace due to the crystal field, the (111)-type combinations of Γ_5 octupoles are the best candidates for octupolar order parameters. Octupolar ordering induces the experimentally

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observed Γ_5-type quadrupoles as secondary order parameters. We studied the effect of an external magnetic field on ferro-octupolar ordering. We found that octupolar order survives up to a critical magnetic field if the field is lying in specific directions, while for general field directions, the underlying symmetry of the model is destroyed and therefore the phase transition suppressed even in weak fields. On the basis of a group-theoretical analysis of the Helmholtz potential we discussed the field-induced multipoles and the field-induced couplings between various order parameters.

We have investigated the collective modes, and the effect of randomly distributed impurities on the transport properties of **unconventional density waves** (UDW) in quasi one dimensional systems. The temperature dependence of the threshold electric field of nonlinear conductivity was calculated in the presence of imperfect nesting, and in an applied magnetic field. 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, and the Nernst effect based on our model. We have calculated the frequency dependent conductivity of the **unconventional superconductor** Sr_2RuO_4, and explored the possibility of a d-UDW in the pseudogap phase of underdoped high-T_c superconductors. Our findings reproduce the experimental results for the angular dependent magnetoresistance and optical dichroism.

From the photoemission (ARPES) data of the high temperature superconductor BiSCO, in the RPA approximation, we calculated the Raman and infrared properties. The results of this single particle approximation are in very good agreement with the measured spectra.

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Levente Vitos	lv@szfki.hu

Grants and international cooperations

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

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

ESF Programme towards atomistic materials design (J. Kollár, 2003-2007)

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. Dóra* B, Maki* K, Virosztek A; Imperfect nesting and transport properties in unconventional density waves; *Phys Rev B*; **66**, 165116/1-8, 2002

C.2. Dóra* B, Maki* K, Korin-Hamzić* B, Basletić* M, Virosztek A, Kartsovnik* MV, Müller* H; The angular dependent magnetoresistance in α-(BEDT-TTF)$_2$KHg(SCN)$_4$; *Europhys Lett*; **60**, 737-742, 2002

C.3. Maki* K, Dóra* B, Virosztek A; Unconventional density wave in the pseudogap phase of high T_c cuprates; *J Physique IV*; **12**, Pr9-45-48, 2002

C.4. Maki* K, Dóra* B, Korin-Hamzić* B, Basletić* M, Virosztek A, Kartsovnik MV; Brave new world of unconventional density waves; *J Physique IV*; **12**, Pr9-49-52, 2002

C.5. Vitos L, Korzhavyi* PA, Johansson* B; Stainless steel optimization from quantum mechanical calculations; *Nature Materials*; **2**, 25-28, 2003

C.6. Dubrovinsky* L, Dubrovinskaia* N, Langenhorst* F, Dobson* D, Rubie* D, Gesmann* C, Abrikosov* I, Baykov* VI, Vitos L, Johansson* B, Le Bihan* T, Crichton* WA; Iron-silica interaction at extreme conditions and the nature of the electrically conducting layer at the base of Earth's mantle; *Nature*; **422**, 58-61, 2003

C.7. Olsson* P, Abrikosov* IA, Vitos L, Wallenius* J; *Ab initio* formation energies of Fe-Cr alloys; *J of Nuclear Materials*; **321**, 84-90, 2003

C.8. Chioncel* L, Vitos L, Abrikosov* IA, Kollár J, Katsnelson* MI, Lichtenstein* AI; *Ab initio* electronic structure calculations of correlated systems; *Phys Rev B;* **67**, 235106, 2003

C.9. Johansson* B, Vitos L, Korzhavyi* PA; Chemical composition-elastic property maps of austenitic stainless steels; *Solid State Scien*ces; **5**, 931-936, 2003

C.10. Barisic* N, Forró* L, Mandrus* D, Jin* R, He* J, Fazekas P; Electrical properties of $Cd_2Re_2O_7$ under pressure; *Phys Rev B*; **67**, 245112/1-8, 2003

C.11. Kiss A, Fazekas P; Quadrupolar interactions in Pr compounds: $PrFe_4P_{12}$ and $PrBa_2Cu_3O_6$; *J Phys-Cond Mat*; **15**, S2109-S2117, Sp. Iss. SI JUL 23 2003

C.12. Dóra* B, Virosztek A, Maki* K; Unconventional spin density wave in the pseudogap phase in high T_c cuprates?; *Acta Phys Pol B*; **34**, 571-574, 2003

C.13. .Dóra* B, Virosztek A; Collective modes in unconventional density waves; *Europhys Lett*; **61**, 396-402, 2003

C.14. Dóra* B, Maki* K, Virosztek A; Optical conductivity of superconducting Sr_2RuO_4; *Europhys Lett;* **62**, 426-432, 2003

C.15. Maki* K, Dóra* B, Kartsovnik* MV, Virosztek A, Korin-Hamzić* B, Basletić* M; Unconventional charge density wave in the organic conductor α-(BEDT-TTF)$_2$KHg(SCN)$_4$; *Phys Rev Lett*; **90**, 256402/4; 2003

C.16 Virosztek A, Dóra* B, Maki* K; Unconventional density waves in organic conductors; *Synth Metals*; **139**, 317-319, 2003

C.17. Dóra* B, Virosztek A, Maki* K; Impurity effects in unconventional density waves in the unitary limit; *Phys Rev B*; **68**, 075104, 2003

C.18. Kollár J, Vitos L, Osorio-Guillén* JM, Ahuja* R; Calculation of surface stress for fcc transition metals; *Phys Rev B*; accepted for publication

C.19. Vitos L,. Korzhavyi* PA, Johansson* B; Austenitic stainless steels from quantum mechanical calculations; *Advanced Engineering Materials*; accepted for publication

C.20. Magyari-Köpe B, Vitos L, Grimvall* G; Anomalous behavior of lattice parameters and elastic constants in hcp Ag-Zn alloys; *Phys Rev Lett*; accepted for publication

C.21. Kiss A, Fazekas P; Octupolar ordering of Gamma8 ions in magnetic field; *Phys Rev B*; accepted for publication

C.22. Dóra* B, Maki* K, Ványolos* A, Virosztek A; Magnetothermopower and Nernst effect in unconventional charge density waves; Phys Rev B (cond-mat/0308335); accepted for publication

Conference proceedings

C.23. Dóra* B, Virosztek A, Maki* K; How to detect unconventional density waves?; In: *Lectures on the physics of highly correlated electron systems VII.*, eds.: A. Avella and F. Mancini, AIP Conf. Proc. **678**, p. 273, Melville, N.Y., 2003

C.24. Vitos L, Abrikosov* IA, Johansson* B; Coherent Potential Approximation within the Exact Muffin-Tin Orbitals Theory; In: *Proceedings of IAC-3 conference;* accepted for publication

Book chapter

C.25. Vitos L; Quantum-mechanical description of substitutional random alloys; In: *Recent Research Developments in Physics*; American Technical Publisher Ltd., 2003

C.26. Fazekas P, Kiss A; Competition and coexistence of magnetic and quadrupolar ordering; In: *Correlated Electrons;* Eds. V. Zlatic and A. Hewson; Kluwer Scientific Publishers, Dordrecht, 2003

See also A.2.

D. NON-EQUILIBRIUM ALLOYS

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

Intermixing of insoluble elements in Fe/Ag granules. — Fe/Ag granular alloys were prepared in the form of discontinuous multilayers by vacuum evaporation of the elements. The samples show superparamagnetic behaviour and the blocking temperatures measured by SQUID magnetometry and Mössbauer spectroscopy, respectively, vary between 12 K and 300 K. The results indicate that the average grain size of the magnetic particles can be modified by changing the amount of the sequentially depositied material (i.e. nominal layer thickness). The Mössbauer measurements indicate that the magnetic grains are not pure bcc-Fe grains despite that Fe and Ag have a large positive heat of mixing, i.e. insoluble in equilibrium. The Fe hyperfine fields measured at 4.2 K show a broad distribution that is associated to a distribution of the number of Ag neighbors around the Fe atoms. The large positive isomer shifts and the observed quadrupole splittings also support this explanation. Broad distribution of hyperfine fields may result from superparamagnetic relaxation of small particles. Since the shape of the distributions remain unchanged in external magnetic fields upto 7 T, this possibility is ruled out. Granular alloys with a distribution in the grain size of the particles are inherently magnetically heterogeneous systems around the average blocking temperature: they behave like ferromagnets below the blocking temperature and superparamagnets above it. The sample preparation by sequential deposition makes it possible to introduce magnetic heterogeneity in a controlled manner. Samples can be designed to contain superparamagnetic and ferromagnetic particles with a well-defined distance and ratio of the magnetically different layers. The magnetoresistance measurements performed at the Budapest University of Technology and Economics indicate that the injection of spin polarized electrons from the ferromagnetic layers can enhance the magnetoresistance of the superparamagnetic granules.

Low-temperature spin freezing in soft magnetic nanocrystalline alloys. — In nanocrystalline alloys produced by controlled crystallization of amorphous ribbons low-temperature spin freezing is observed. It is often attributed to the spin-glass behaviour of the ferromagnetic grain boundaries. On the contrary, our investigation shows that it is connected to the dynamical behaviour of individual grains decoupled from the ferromagnetic matrix. This phenomenon observed below 25 K was studied in the nanocrystalline (nc)-$Fe_{92-x}Zr_7B_xCu_1$ (x = 2-21 at%) alloy series. The freezing causes magnetic hardening with increasing B concentration and annealing temperature (which determines the amount of nanocrystals), as it is shown by the temperature dependence of both the susceptibility and coercive field. The temperature dependence of the relative change of magnetization, M(rel), normalized to M_{FC} (5K) is plotted in Figs. 1 and 2 for different boron contents, x and for different amounts of nanocrystals in nc-$Fe_{80}Zr_7B_{12}Cu_1$, together with the corresponding curves for the coercive field (H_c). Both quantities indicate increasing magnetic hardening with increasing boron content and with the nanocrystalline fraction. At low temperatures H_c is determined dominantly by the blocking of decoupled clusters whereas above 50 K the remaining small H_c is characteristic of domain wall pinning. A rough estimate of the average blocking temperature of the clusters, T_B = 20 K, taken as the inflection point of the magnetization curves measured for applied magnetic fields, $H_m \rightarrow 0$, leads to an average cluster size (D) of around 6 nm for nc-$Fe_{74}Zr_7B_{18}Cu_1$ with the assumption of the anisotropy constant of bcc Fe ($K = 4.8 \times 10^4$ J/m^3). Both the magnitude of the deviation of the FC (field cooling) and ZFC (zero-field cooling) curves at T = 5 K and H_c seem to be proportional to T_B, i.e. to the magnetic anisotropy and particle volume. The observed phenomenon is

attributed to the gradual magnetic blocking of a fraction of nanocrystals decoupled from the ferromagnetic matrix.

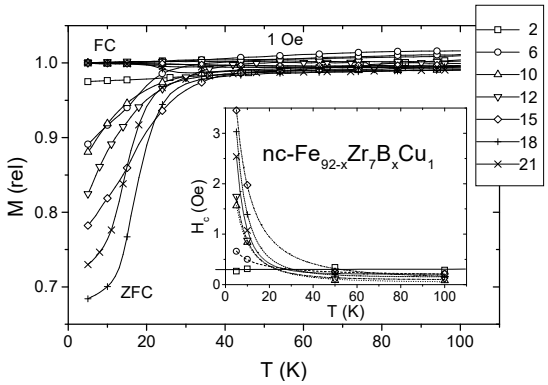

Fig. 1. Temperature dependence of the relative change of magnetization for fully (100%) nc-$Fe_{92-x}Zr_7B_xCu_1$ alloy series (x = 2-21 at%) after ZFC and FC for measuring and cooling field of 1 Oe. Inset: same for the coercive field. The lines are guides to the eye.

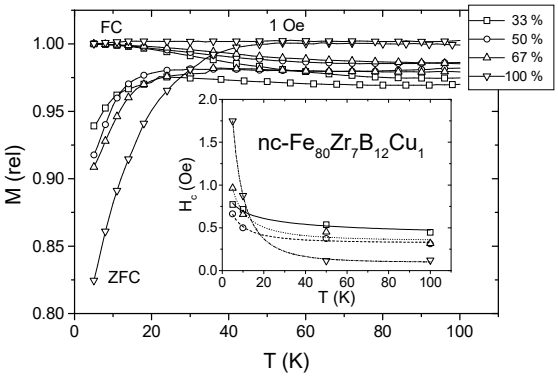

Fig. 2. Temperature dependence of the relative change of magnetization for nc-$Fe_{80}Zr_7B_{12}Cu_1$ alloy annealed to a degree of 33%, 50%, 67% and 100% of the nc state after ZFC and FC for measuring and cooling field of 1Oe. Inset: same for the coercive field. The lines are guides to the eye.

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Grants and international cooperations

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:

— Javier Sebastián Blázquez-Gámez, Dpto. Fisica de la Materia Condensada, ICMSE CSIC Univ.Sevilla, Oct.-Nov. 2003, Host: L.F. Kiss

Publications

Articles

D.1 Gavrilenko* KS, Vértes* A, Vanko* G, Kiss LF, Addison* AW, Weyhermüller* T, Pavlishchuk* VV; Synthesis, magnetochemistry, and spectroscopy of heterometallic trinuclear basic trifluoroacetates $[Fe_2M(\mu_3\text{-}O)(CF_3COO)_6(H_2O)_3]\bullet H_2O$ (M = Mn, Co, Ni); *Eur J Inorg Chem*; 3347-3355, 2002

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D.7. Lukáčová* M, Kiss LF, Maryško* M, Mihalik* M, Mitróová* Z, Stopka* J, Zentko* A, Zentková* M; New magnetic phenomena in vanadium hexacyanochromates; *Phys Stat Sol (a)*; **196**, 240-243, 2003

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D.9. Kemény T, Kiss LF, Kaptás D, Balogh J, Bujdosó L, Gubicza* J, Vincze I; Superparamagnetic behaviour of $Fe_{80}B_{12}Zr_7Cu$ alloys with different fractions of primary nanocrystalline phase; *Mater Sci Eng A*; accepted for publication

D.10. Lovas* A, Böhönyey* A, Kiss LF, Kováč* J, Németh* P; Some new results on amorphous Curie-temperature relaxation; *Mater Sci Eng A*; accepted for publication

D.11. Juhász* R, Cziráki* Á, Kiss LF, Lovas* A; Stress sensitivity and nanocrystalline phase evolution in Finemet-type alloys; *Mater Sci Eng A*; accepted for publication

D.12. Mihály* L, Talbayev* D, Kiss LF, Zhou* JS, Fehér* T, Jánossy* A; Field-frequency mapping of the electron spin resonance in the paramagnetic and antiferromagnetic states of $LaMnO_3$; *Phys Rev B*; accepted for publication

D.13. Gál* M, Kiss LF, Klencsár* Z, Pápai* I, Schubert* G, Rohonczy* J, Vértes* A, Wagner* FE; Mössbauer, magnetization and nuclear magnetic resonance measurements and

DFT calculations on some iridium (I) complexes with fullerene ligands; *J Radioanal Nucl Chem*; accepted for publication

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Book chapter

D.17 Balogh J, Kaptás D, Kiss LF, Kemény T, Temst* K, Van Haesendonck* C, Vincze I; Mössbauer study of Fe grains in nanocomposites; *NATO ARW Series*; Kluwer Academic Publ., accepted for publication

See also H.11.

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 related systems. — The fullerenes are closed shell all carbon atom molecules. The most abundant among them is the C_{60} molecule.

Fullerenes can form a large variety of compounds with elements or with other molecules. In the group of A_xC_{60} compounds (A=Na, K, Rb, Cs) there are materials with very interesting properties. Many superconducting materials (A_3C_{60}), and also polymers with different dimensionality (RbC_{60}, Na_4C_{60}) were found. Beside the above examples, the charge transfer from the alkali metals to the C_{60} leads to various interesting effects. Among them we investigated the Jahn-Teller distortion (JTD) in A_4C_{60} (A=K, Rb, Cs) and Na_2C_{60}. At low temperature a static JTD while at high temperature a dynamic JTD was found in the A_4C_{60} compounds. The behavior of the Na_2C_{60} differs from the A_4C_{60} type samples. At low temperature there is a nanoscale segregation to Na rich and C_{60} rich regions, while at high temperature a dynamic JTD can be deduced. An other interesting system related to C_{60} is the $(C_{59}N)_2$. However, the synthesis of this material is not fully understood. Two methods were published, both with very low efficiency and no clear reproducibility. We worked out a new synthetic route with higher efficiency. The adaptation of this method to larger quantities is under way.

Similarly to the fullerene molecules, carbon nanotubes are also exclusively built from carbon atoms. In a joint work with scientists from the University of California we studied the bond formation of single-walled carbon nanotubes (SWNTs). Since these materials are the only carbon-based metals, they provide a unique opportunity to explore the effect of carbon-carbon bond formation at the surface of a metal. We showed that adding dichlorocarbene substitutents to the walls of the SWNTs the conversion of conjugated sp^2 bonds into saturated sp^3 bonds brings about a very strong suppression of the spectral weight at the Fermi level. This is a unique manifestation of the chemistry of carbon nanotubes, and it is a clear point of differentiation from the behavior seen with ionic chemistry.

Atomic resolution imaging of small clusters by hard x-ray free electron lasers. — Two hard x-ray Free Electron Lasers (FEL) are under construction: one in Hamburg and the other in Standford. These x-ray sources will give unprecedented intensities and in very short pulses. These unique features will allow totally new measurements leading to a deeper understanding of various phenomena in many areas of science. One of these areas is the structure determination. Presently, the bottleneck in structure determination is the need for crystalline samples. Based on the idea of Janos Hajdu (University of Uppsala) this could be avoided by collecting data on the structure of a single molecule or atom cluster during a single pulse, before the radiation damage could occur. To assess the feasibility of this type of measurements one has to know how a small cluster of atoms behaves in the very intense and rapidly oscillating electromagnetic field. This can be found out from model calculations only, since no experiments can be done with available sources. We developed a model, which describes the behavior of a cluster of carbon atoms in the x-ray FEL pulse. It was found that the cluster Coulomb explodes. Analyzing the dynamics of the explosion we showed that useful structural data can only be collected in the first part of a pulse. Using a special reconstructing algorithm we could invert the continuous elastic scattering pattern to

[#] Ph.D. student

real space structure. Beside the feasibility of structure determination our calculations give an insight to the physics of cluster explosion (Fig.1.).

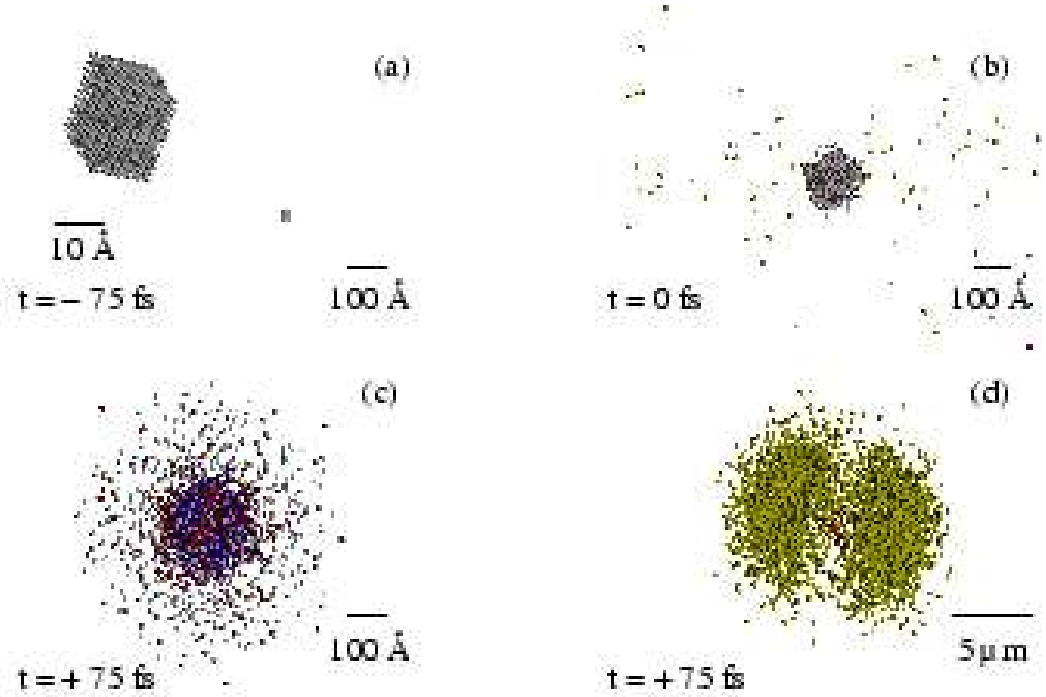

Fig.1. Snapshots of the explosion of a 1500 carbon atom cluster in the XFEL beam. –75 fs is the beginning of the gaussian pulse, zero fs is the maximum and 75 fs is the end of the pulse.

Theory of phase transformations. — The phase field theory of crystal nucleation developed earlier has been applied for nucleation in hard-sphere liquids. The exact thermodynamics from molecular dynamics is used. The interface thickness for phase field is evaluated from the cross-interfacial variation of the height of the singlet density peaks. The model parameters are fixed in equilibrium so that the free energy and thickness of the (111), (110), and (100) interfaces from molecular dynamics are recovered. Assuming spherical symmetry, we evaluate the height of the nucleation barrier and the Tolman length without adjustable parameters. The barrier heights calculated with the properties of the (111) and (110) interfaces envelope the Monte Carlo results, while those obtained with the average interface properties fall very close to the exact values. In contrast, the classical sharp interface model considerably underestimates the height of the nucleation barrier. We find that the Tolman length is positive for small clusters and decreases with increasing size, a trend consistent with computer simulations.

Recent observations on clay-polymer blend films indicate that particulate additives, in addition to serving as nucleating agents, may also perturb crystal growth, leading to the formation of irregular dendritic morphologies. We have described the formation of these "dizzy dendrites" using a phase field theory in which randomly distributed foreign particle inclusions perturb the crystallization by deflecting the tips of the growing dendrite arms (Fig.2.). This mechanism of crystallization, which has been verified experimentally, leads to a polycrystalline structure dependent on particle configuration and orientation. Using computer simulations we have demonstrated that additives of controlled crystal orientation should allow for a substantial manipulation of the crystallization morphology.

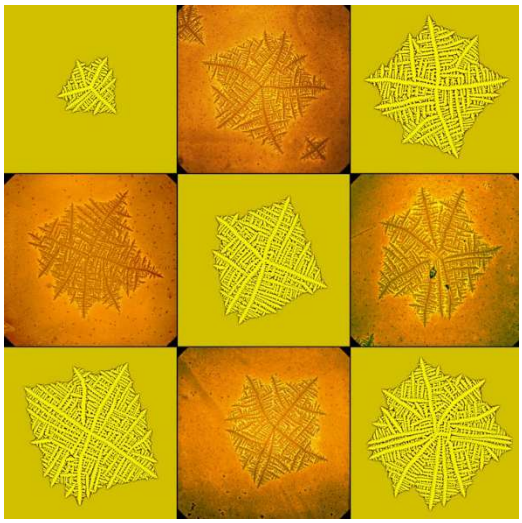

Fig. 2. 'Dizzy' dendrites formed by sequential deflection of dendrite tips on foreign particles: Comparison of experiments on 80 nm clay-polymer blend film (darker panels, by the courtesy of V. Ferreiro and J. F. Douglas) and phase field simulations (lighter panels). The simulations have been selected from 30 random configurations according to their resemblance to the experimental patterns. (The simulations were performed on a 3,000×3,000 grid, with 18,000 orientation pinning centers per frame.)

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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).

ESA Prodex 90109 Phase field modelling of peritectic solidification (L. Gránásy, 2003)

OTKA T043237 Elastic x-ray scattering in structural research (G. Faigel 2003-2005)

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)

Publications

Articles

E.1. Gránásy L, Pusztai T; Diffuse interface analysis of crystal nucleation in hard-sphere liquid; *J Che*m *Phys*; **117**, 11121-11124, 2002

E.2. Tegze M, Faigel G, and Marchesini* S; Comment on "X-ray absorption holography"; *Phys Rev Lett*; **89**, 279601, 2002

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E.10. Zhu* Z-T, Musfeldt* JL, Kamarás K, Adams* GB, Page* JB, Kashevarova* LS, Rakhmanina* AV, Davydov* VA; Far-infrared vibrational properties of linear C_{60} polymers: A comparison between neutral and charged materials; *Phys Rev B*; **67**, 045409, 1-9, 2003

E.11. Kamarás K, Itkis* ME, Hu* H, Zhao* B, Haddon* RC; Chemistry at the Fermi level: covalent bond formation to a carbon nanotube metal; *Science*; **301**, 1501, 2003

E.12. Deák* P, Gali* A, Sólyom* A, Ordejón* P, Kamarás K, Battistig* G; Studies of boron-interstitial clusters in Si; *J Phys Condens Matter*; **15**, 4967-4977, 2003

E.13. Hu* H, Zhao* B, Hamon* MA, Kamarás K, Itkis* ME, Haddon* RC; Sidewall functionalization of single-walled carbon nanotubes by addition of dichlorocarbene; *J Am Chem Soc;* accepted for publication

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E.14. Warren* JA, Loginova* I, Gránásy L, Börzsönyi T, Pusztai T; Phase field modeling of alloy polycrystals ; In: *Proceedings of the Modeling of Casting, Welding and Advanced Solidification Processes*; Eds.: D. Stefanescu et al., TMS Publications; pp. 45-52, 2003

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E.16. Kováts É; Pekker S; Fullerene Photopolymer; In: *Proceedings of the XVIIth International Winterschool on Electronic Properties of Novel Materials, Kirchberg, Austria, March 8-15, 2003*; Eds.: H. Kuzmany et al, AIP Conference Proceedings, Vol **685**; pp.46-49. 2003

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Book chapters

E.18. Gránásy L, Börzsönyi T, Pusztai T; Phase field theory of nucleation and growth in binary alloys; Interface and Transport Dynamics; In: *Computational Modelling, Lecture Notes in Computational Science and Engineering;* Eds.: H. Emmerich, et al., Springer, Berlin; vol. **32**, pp. 190-195, 2003,

E.19. Gránásy L, Pusztai T, Börzsönyi T, James* PF; Continuum models for crystal nucleation in undercooled melts and glasses; In: *Nucleation Control*; Eds.: G.W. Greenwood, A.L. Greer, D.M. Herlach, K.F. Kelton, Camb. Univ. Press, Cambridge, 2003, accepted for publication.

F. ELECTRON CRYSTALS

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

Dissipation in High-T_c superconductors. — Understanding dissipative processes in superconductors is both a theoretical challenge and a question of paramount importance for applications. In "classical" superconductors, dissipation in response to slowly varying electromagnetic fields is dominated by the dynamics of Abrikosov vortices. In high-critical-temperature (high-T_c) superconductors another mechanism of comparable importance is the Josephson tunneling between conducting layers. We have conducted extensive transport measurements with current in excess of the resistive breakdown in suitably patterned single crystals of the high-T_c superconductor $Bi_2Sr_2CaCu_2O_8$ with the aim of determining the source of dissipation under a broad range of magnetic fields and temperatures. We have concluded that in each case, the breakdown is a simultaneous effect of both mechanisms. Dissipation arises in a region localized in space to the neighborhood of current injection. We have traced the increase of dissipative volume with increasing current.

Nuclear magnetic resonance in fullerides. — The physical properties of the alkali metal fullerides A_nC_{60} are to a large extent dependent on the orientational order of the C_{60} molecules in the solid. Nuclear magnetic resonance (NMR) is a sensitive local probe of the orientational order as well as of the dynamics of reorientation. We have measured the ^{23}Na NMR spectrum and relaxation in Na_2CsC_{60} in order to clarify some long-standing problems in the broad class of alkali fullerides. We have shown that the NMR spectrum splits at low temperatures and this splitting is correlated with the broadening of the ^{13}C spectrum. We propose that the different ^{23}Na NMR lines correspond to different fullerene orientational environments of the tetrahedral alkaline site.

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Grants and international cooperations

OTKA T037976	Dissipation in type-II superconductors (G. Kriza, 2002-2004)
OTKA TS040878	Collective electronic states in solids (SZFKI[2] principal investigator: G. Kriza, 2002-2004)

Long term visitors

— F.I.B. Williams, Service de Physique de l'État Condensé, Commissariat à l'Energie Atomique, Saclay, France; February to April 2003 (KFKI-CMRC grant; host: G. Kriza)

[#] *Ph.D. student*

[2] SZFKI: Hungarian acronym of the Research Institute for Solid State Physics and Optics

Publications

Articles

F.1. Clark* WG, Tanaka* KB, Vonlanthen* P, Kriza G; New insights on charge density wave and other fluctuations in blue bronze from NMR measurements; *J Phys (France) IV*; **12**, Pr9/365-368, 2002

F.2 Pethes I, Pomar* A, Sas B, Kriza G, Vad* K, Pallinger Á, Portier* F, Williams* FIB; Potential and current distribution in strongly anisotropic $Bi_2Sr_2CaCu_2O_8$ single crystals at current breakdown; *Phys Rev B*; **68**, 184509/1-9, 2003

F.3 Matus P, Alloul* H, Singer* PM, Brouet* V, Kriza G, Garaj* S, Forró* L; Fullerene local order in Na_2CsC_{60} by ^{23}Na NMR; *Appl Magn Res;* accepted for publication

G. LIQUID CRYSTALS

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

Electroconvection in an unusual nematic compound with strongly positive dielectric anisotropy and negative anisotropy of the conductivity has been investigated. For homeotropic alignment, where one has a direct transition to rolls or squares depending on the frequency of the applied voltage (Fig.1.), we have presented a quantitative theory. From the comparison we have inferred values for some viscosities, which are rather unusual, but not unreasonable in view of the vicinity of the nematic-smectic transition. For planar alignment, electroconvection sets in above a splay Freedericksz transition with "parallel rolls," which is also captured by the theory.

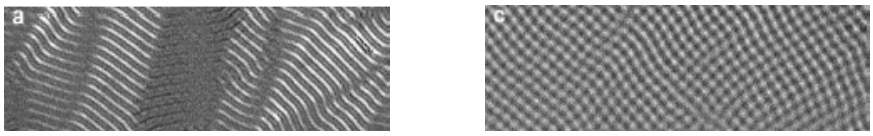

Fig.1. Electroconvection patterns in a nematic: rolls and squares.

The influence of an external electric field (applied to the nematic liquid crystal layer) on the morphology of the **nematic liquid crystal – air interface** has been studied experimentally in radial Hele-Shaw geometry. The effective viscosity μ_{eff} of the nematic has been tuned by the electric field E and by the flow. At low excess pressure p_e (where the growth of the interface is controlled mainly by the surface tension σ), the applied E has no significant influence on the morphology of the interface, but decreases its normal velocity due to the increase of μ_{eff}. At higher p_e (where the growth is controlled not only by σ, but also by the kinetic term that depends on the effective viscosity) a significant difference in the morphology has been observed as a function of E (Fig.2.). Experiments have shown that the influence of the electric field on the pattern morphology increases with the driving force (pressure gradient).

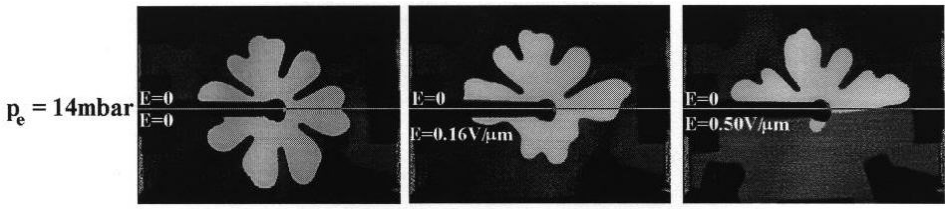

Fig.2. Supression of the growth of viscous fingers by electric field.

Our calculations have proved that an anticlinic arrangement with 45° tilt angle and with 109.5° opening angle of bent-shape molecules results in an **optically isotropic antiferroelectric smectic structure** that can be reversibly switched to birefringent states. Experimentally we have found that an ester based banana-shape substance synthesized in our laboratory almost fulfils the ideal conditions and provides fast electro-optical switching with or without crossed polarizers. Antiferroelectric anticlinic bent-core liquid crystals with the above calculated 'ideal' parameters can be used in displays, which provide sub-millisecond switching and very wide viewing angle without the need of precise uniform

[#] *Ph.D. student*

alignment control. These features hold for both scattering type (without polarizers) and electrically controllable birefringent (with polarizers) displays.

The **light-induced anisotropy** has been measured in dye-doped high-viscosity fluids (glycerin, glucose) using low power lasers. The temperature dependence showed a critical slowing down around the glassy transition. In azo-dye doped liquid crystals, we have shown that the reorientational optical nonlinearity changes sign as a function of intensity.

Studies of the **alignment of liquid crystals on soft polymer surfaces** have shown that they mutally affect each other's structure. This effect has been captured both in the kinetics of photoalignment and in the relaxation of twist angles in magnetically induced twisted nematic cells.

New **banana-shaped liquid crystalline monomers** (dienes) have been prepared (Fig.3. A). These compounds have been used as building blocks in a polycondensation reaction by reacting nematic diacrylates (Fig.3. B) with the above dienes using alternating diene methathesis polymerization (ALTMET) reaction. These products are the very first examples of such main-chain liquid crystalline polymers where the banana shaped monomers were reacted with rod-like ones leading to the formation of perfectly alternating ...ABABAB... type copolymers. This novel method is very versatile and allows preparation of copolymers of diverse structures. The physico-chemical and electro-optical properties of the new derivatives are under investigation. According to the preliminary results, the polymer preserved the nematic properties of the monomers.

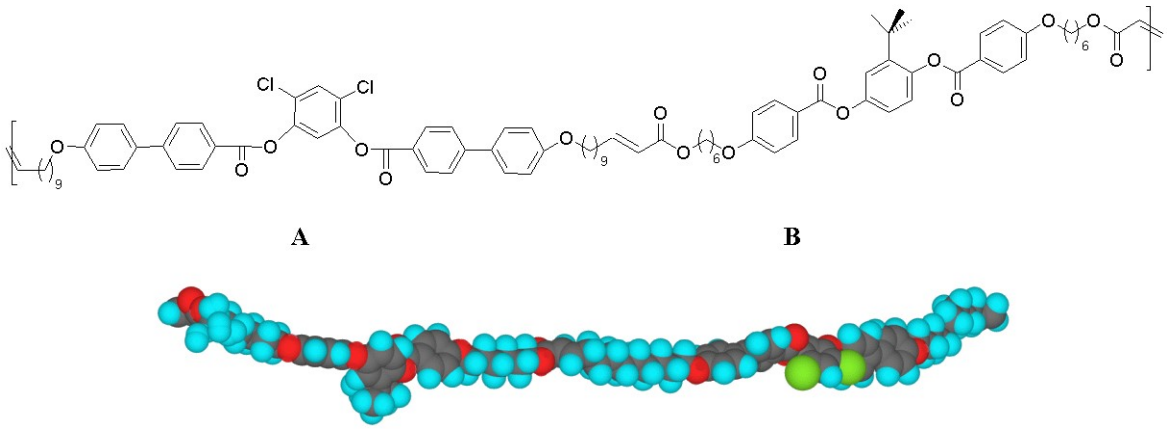

Fig.3. Structural formula and space filling model of the building unit of the copolymer.

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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, 1999-2003)

OTKA T-031808 Convective and interfacial instabilities in liquid crystals. (Á. 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. (K. Fodor-Csorba, 2000-2003)

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

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

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

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

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

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

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

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

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

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. (Á. Buka, 2002-2005)

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

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

NATO PST.ASI.979405 Pattern formation, granular physics and soft condensed matter. (Á. Buka, 2002-2003)

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

Long term visitors

— Lorenz Kramer: University of Bayreuth, Bayreuth, Germany, 15 March-15 April, 2003, (KFKI-CMRC grant, host: Á. Buka and N. Éber).

— Shankar Rao: Centre for Liquid Crystal Research, Bangalore, India, 15 Juni-15 August, 2003, (INSA-HAS exchange program, host: I. Jánossy).

— Marta Becchi: Technical University of Torino, Torino, Italy, 1 July- 31 July, 2003, (KFKI-CMRC grant, host: I. Jánossy).

— David Statman: Alleghiny College, Meadville, Pennsylvania, USA, 1 June-30 June, 2003, (host: I. Jánossy).

— Elzbieta Kochowska: The Henryk Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences, Cracow, Poland, 1 Januar- 31 December, 2003, (EU-RTN grant, host: Á. Buka).

— Wojcziech Otowski: Cracow University of Technology, Cracow, Poland, 1 November-30 November, 2003, (KFKI-CMRC grant, host: Á. Buka).

Publications

Articles

G.1. Buka Á, Dressel* B, Otowski* W, Camara* K, Tóth-Katona T, Kramer* L, Lindau* J, Pelzl* G, Pesch* W; Electroconvection in nematic liquid crystals with positive dielectric and negative conductivity anisotropy; *Phys Rev E;* **66**, 051713/1-8, 2002

G.2. Stojadinovic* S, Adorjan* A, Sprunt* S, Sawade* H, Jákli A; Dynamics of the nematic phase of a bent core liquid crystal; *Phys Rev E;* **66,** 060701(R)/1-4, 2002

G.3. A. Jákli, Toledano* P; Unusual sequences of tilted smectic phases in liquid crystals of bent-shape molecules; *Phys Rev Lett;* **89**, 275504/1-4, 2002

G.4. Jákli A, Nair* GG, Sawade* H, Heppke* G; A bent-shape liquid crystal compound with antiferroelectric triclinic-monoclinic phase transistion; *Liquid Crystals;* **30**, 265-271, 2003

G.5. Mátyus* E, Fodor-Csorba K; Synthesis and liquid crystal properties of new banana-shaped cinnamoyl derivatives; *Liquid Crystals;* **30,** 445-450, 2003

G.6. Tóth-Katona T, Buka Á: Nematic-liquid-crystal-air interface in a radial Hele-Shaw cell: Electric field effects; *Phys Rev E;* **67**, 041717/1-7, 2003

G.7. Tóth Katona T, Cressman* JR, Goldburg* WI, Gleeson* JT; Persistent global power fluctuations near a dynamic transition in electroconvection, *Phys Rev E;* **68**, 030101(R)/1-4, 2003

G.8. Jánossy I, Benkler* E; Light-induced dichroism and birefringence in dye-doped glycerin; *Europhys Lett;* **62,** 698-704, 2003

G.9. Statman* D, Jánossy I; Study of photoisomerization of azo dyes in liquid crystals; *J Chem Phys;* **118,** 3222-3232, 2003

G.10. Jánossy I; Photo-orientation at liquid crystal – polymer interfaces; *Pramana*; **61**, 435-445, 2003

G.11. Demel* S, Slugovc* C, Stelzer* F, Fodor-Csorba K, Galli* G; Alternating diene metathesis polycondensation (ALTMET) – a versatile tool for the preparation of perfectly alternating AB copolymers. *Macromol Rapid Comm;* **24**, 636-641, 2003

G.12. Jákli A, Huang* YM, Fodor-Csorba K, Vajda A, Galli* G, Diele* S, Pelzl* G; Reversible switching between optically and birefringent states in a bent-core liquid crystal; *Adv Mater;* **15**, 1606-1610, 2003

G.13. Tóth Katona T, Gleeson* JT; Conductive and dielectric defects, and anisotropic and isotropic turbulence in liquid crystals – electric power fluctuation measurements; *Phys Rev E;* **68**, accepted for publication

G.14. Tóth Katona T, Gleeson* JT; Power fluctuations in electroconvection – probability density function forms; *Phys Rev Lett;* accepted for publication

Conference proceedings

G.15. Jákli A, Chien* LC, Krüerke* D, Rauch* S, Sawade* H, Bault* P, Heppke* G, Fodor-Csorba K, Nair* GG; Light shutters and electro-optical storage devices from antiferroelectric liquid crystals of bent-shape molecules; In: *Electronic Imaging: Liquid crystal Materials, Devices and Applications, IX, Santa Clara, Proc. SPIE*, Vol. **5003**, 74-80, 2003

G.16. Jákli A, Fodor-Csorba K; Electro-optics of liquid crystals of bent-shape molecules; In: *Proc. of 3rd International Meeting on Information Display, Seoul, Aug. 2003;* pp 1108-1111, 2003

Book chapter

G.17. Börzsönyi T, Akamatsu* S, Faivre* G; Dynamics of a faceted nematic-smectic B front in thin sample directional solidification; In: *Interface and transport dynamics, Lecture Notes in Computational Science and Engineering;* Eds.: H.Emmerich, B.Nestler and M.Schreckenberg, Springer, Vol 32, 166, 2003

G.18. Garic* C, Obadovic* DZ, Bubnov* A, Hamplova* V, Kaspar* M, Vajda A, Fodor-Csorba K, Éber N; Physical characterisation of the ferroelectric liquid crystalline mixture; In: *Proc. of the Fifth General Conference of the Balkan Physical Union BPU-5*, *Vrnjacka Banja, August 25-29 2003*; Serbian Physical Society, Belgrade, 2003

See also E.4, E.14., E.18., 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. — High purity Pd and Pd_{1-x}-Ag_x (x = 0.1, 0.2, 0.25 and 0.35) alloys were charged and discharged with hydrogen, and the NMR free induction decay (FID), different echoes, T_1 and $T_{1\rho}$ spin-lattice relaxation times in the laboratory and rotating reference systems, respectively, were measured in a broad temperature range down to 2.4 K on these fcc crystalline alloys which represent a model material for a chemically disordered system for hydrogen storage materials. Samples with H/M = 0.04…0.7 hydrogen content were prepared and investigated. The explicit frequency dependence of T_1 and $T_{1\rho}$ below 150 K showed the cross relaxation between proton and quadrupolar palladium-105 nuclear spins. It is the first evidence of this relaxation channel being active in palladium-silver-hydrogen systems. 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 ^{1}H NMR spectrum of unknown origin. In-situ hydrogen charging (discharging) process was also realized in $Pd_{0.75}Ag_{0.25}$–H alloys and simultaneous hydrogen concentration and nuclear spin-spin relaxation time measurements were done. Concentration-gradient driven diffusion coefficient was estimated from the hydrogen concentration-charging (discharging) time curve and data for the intrinsic diffusivity were deduced from the spin-spin relaxation time. Two-component spin-spin relaxation was found in the whole hydrogen concentration range, and one of these contributions is attributed to the hydrogen atoms embedded in the α phase, the other one to those in the β phase at high H concentration (Fig.1.). The diffusion motion is localized up to 10^5-10^6 intrinsic steps and there is no hydrogen atom exchange between the α and β phases on the time scale of spin-spin relaxation.

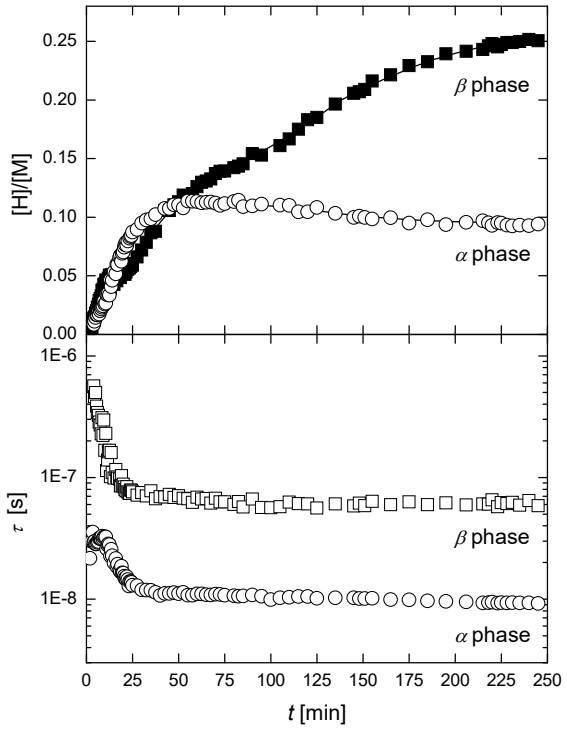

Figure 1. In-situ hydrogen charging process in $Pd_{0.75}Ag_{0.25}$–H alloy. Lower graph: *Correlation times of the intrinsic diffusivity deduced from the spin-spin relaxation time.* Upper graph: *Hydrogen concentrations [H]/[M] in the* α *and the* β *phase.*

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 "π/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 are sensitive and give the quantity of different electric field perturbation ranges existing in this heterogeneous material.

— *Hydrogenated carbon materials.* — Chemically hydrogenated single-wall carbon nanotube, graphite and fullerene samples prepared via a dissolved metal reduction method in liquid ammonia were investigated by ^{1}H NMR. Hydrogen contents were determined from signal intensities. Spectra of different type echo signals and relaxation time were analyzed to characterize the chemically bound hydrogen content.

— *Yttrium aluminum borate $YAl_3(BO_3)_4$.* — ^{11}B NMR spectra were obtained on single and polycrystalline YAB samples: pure and doped with 0.01 Er atom / YAB molecule to characterize the two different boron sites having C_3 and C_2 point symmetry, respectively. The line shifts of single crystals were detected at two different crystal orientations. Axially symmetric electric field gradient tensors of $V_{ZZ} = 2.8$ V/mm^2 were found for both sites. The erbium dopant caused no significant change in the symmetry or value of the electric field gradient tensor at the boron sites.

— *Hydration of semi-structured proteins.* — Temperature dependence of NMR FID signal amplitude, spin-lattice and spin-spin relaxation times of water protons were studied in the physiological solutions of three semi-structured proteins, namely hCSD1, MAP2c and ERD10, moreover as a reference material of structured protein BSA, and the buffer solutions. The steps observed in the measured quantities shows that the mobile ("free") fraction of water freezes at about -6 °C…-12 °C. 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-freezable ("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. The interpretation of the relaxation times with respect to the kinetic characteristics of bound water molecules are in progress (in cooperation with Institutes of Enzymology and Biophysics, Biological Research Center, HAS).

Origin of GMR contributions in electrodeposited multilayers. – It was reported previously that the room-temperature magnetoresistance (MR) curves of Ni-Cu/Cu multilayers electrodeposited by means of current control usually consist of a rapidly varying low-field component up to about 1 kOe and a slowly varying high-field component persisting up to beyond 18 kOe. With the help of detailed magnetic measurements, it has been established recently that besides a normal ferromagnetic (FM) contribution, these multilayers also contain superparamagnetic (SPM) regions. Thus, the magnetic layers can be thought of as breaking up into regions with two different magnetic behaviours. This is mainly the result of the so-called exchange reaction taking place during the deposition of the non-magnetic Cu layer in which process part of the Ni atoms of the previously deposited magnetic layers are removed and replaced by non-magnetic Cu atoms. This random process can lead, in extreme cases, to the formation of isolated magnetic islands, which, due to their small size, may exhibit SPM behaviour. The consequences of the exchange reaction on the final appearance of the magnetic layer in the multilayer structure can be visualized as depicted in Fig.2. We have large areas of the magnetic layers which exhibit FM behaviour.

The separating (or decoupling) regions can consists of either pure Cu metal or a Ni-Cu alloy with Ni-content below the critical concentration for the onset of ferromagnetism (about 45 at.% Ni). The orientation of the magnetization in the FM layers lies in the layer plane as indicated in the schematic view of Fig. 2 by the horizontal arrows in the FM layers. The shorter dashed arrows intend to show that the neighbouring layer magnetizations are not necessarily completely parallel or antiparallel. However, just due to the random orientation of the magnetization directions in the sublayer domains, a partial antiparallel alignment of the magnetizations of neighbouring layers may exist in most areas. All this means that electrons travelling from one FM layer to another one through the non-magnetic spacer layer undergo a spin-dependent scattering and will contribute to the observed MR by a usual GMR term (denoted by GMR_{FM}). Due to the random distribution of FM and SPM regions within the magnetic layer plane on both sides of the Cu spacer layer, electrons polarized in a FM region can reach within the spin-memory time also a SPM region. At room temperature (i.e., above the blocking temperature), the SPM moment orientation fluctuates randomly and, therefore, an electron arriving at the SPM region will find, with a great probability, a different local magnetization orientation than its original polarization and will undergo spin-dependent scattering. This contribution to the observed GMR will be denoted as GMR_{SPM}. By the same arguments, we can ascribe a GMR_{SPM} contribution also to those electrons which travel from a SPM region to a FM region or between two SPM regions as indicated in Fig.2. The term GMR_{SPM} can be considered the same as leading to the GMR observed in granular alloys in which only SPM entities represent magnetic regions with their magnetization orientation varying on a scale less than or at most comparable to the mean free path in the non-magnetic metal matrix.

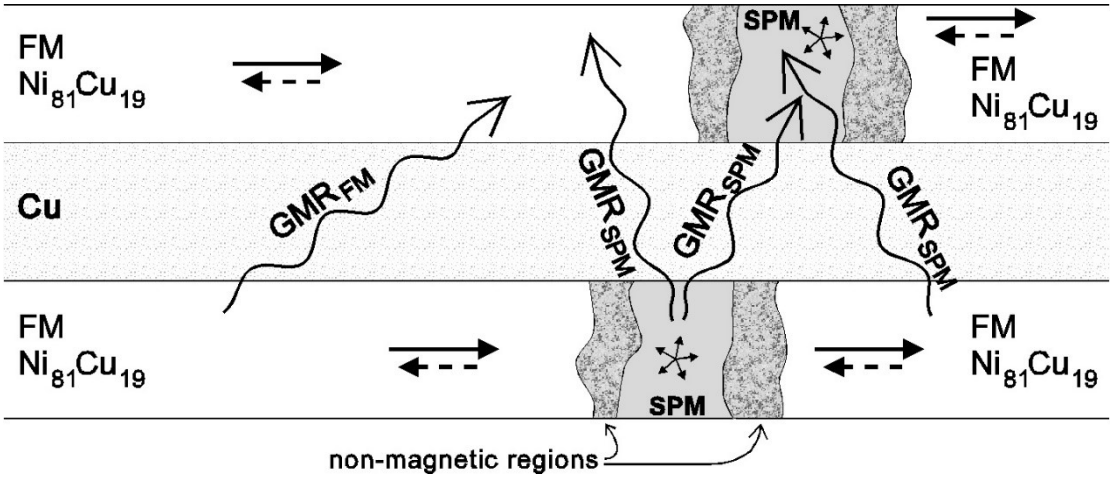

Fig.2. *Schematic view of the room-temperature cross-sectional magnetic profile of electrodeposited Ni-Cu/Cu multilayers with the possible individual GMR contributions*

The total GMR of electrodeposited Ni-Cu/Cu multilayers can be considered as consisting of FM and SPM contributions according to Fig.2.:

$$GMR = a_{FM\text{-}FM}\, GMR_{FM} + (a_{SPM\text{-}SPM} + 2a_{FM\text{-}SPM})\, GMR_{SPM}. \quad (1)$$

The prefactors $a_{FM\text{-}FM}$, $a_{SPM\text{-}SPM}$ and $a_{FM\text{-}SPM}$ have been introduced in order to account for the different interface area fraction of the FM and SPM regions (by assuming that $a_{SPM\text{-}FM} = a_{FM\text{-}SPM}$).

On this basis, we can now identify the low-field and high-field MR contributions by considering the differences in their field dependence. The GMR_{FM} term corresponds to spin-

dependent scattering processes for electrons travelling between two FM regions since this term saturates around technical saturation. The magnetization data indicated that the SPM regions require very high magnetic field for achieving saturation and the same holds for the MR curves. Therefore, the multilayer MR contribution persisting beyond technical saturation (2 to 3 kOe) can be assigned to the magnetically nonsaturated SPM regions of the multilayers which are responsible for the GMR_{SPM} term.

Hydrogen permeation and entrapment kinetics in metals. — By using the results of the theoretical study performed in the last years concerning the impact of entrapment rate on the permeation characteristics, a program was developed to perform a semi-automatic analysis of permeation curves. The program involves the work diagram that makes the connection between parameters obtained from permeation curves and those derived from the theoretical analysis. The program named Permeval guides the user through the entire analysis, supports the user by calculations and takes care of the right order of the calculation and data transformation steps. For permeation experiments, a new electrolyte composition was applied that makes it possible to deposit a Pd layer at the exit side and carry out the entire electrochemical permeation experiment without changing the electrolyte. The application of such an electrolyte substantially shortens the time required by the electrode preparation and facilitates the introduction of the electrochemical permeation method in industrial laboratories. Several hundred steel sheets were examined by the electrochemical permeation techniques. The feasibility of the technique elaborated was obvious. The main conclusion of the experimental work was that the industrial samples are very inhomogeneous; however, the inhomogeneity does not influence the enameling properties.

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Grants

OTKA T 031994 Random walk and diffusion of hydrogen in alloys (K. Tompa, 2000-2003)

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, 2001-2004)

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)

Wellcome Trust ISRF GR067595MA, Study of partially structured protein solutions. Research grant for the Institute of Enzimology of HAS, participant: K. Tompa (2003-2004).

Long term visitor

— Q.X. Liu, Central Iron and Steel Research Institute (CISRI), Beijing, China (Jan. - Dec. 2003; host: I. Bakonyi)

Publications

Articles

H.1. Cziráki* Á, Köteles* M, Péter L, Kupay* Z, Pádár J, Pogány L, Bakonyi I, Uhlemann* M, Herrich* M, Arnold* B, Thomas* J, Bauer* HD, Wetzig* K; Correlation between interface structure and giant magnetoresistance in electrodeposited Co-Cu/Cu multilayers; *Thin Solid Films;* **433**, 237-242, 2003

H.2. 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;* **424**, 229-238, 2003

H.3. Marek* T, Bokor M, Tompa K, Vértes* A, Süvegh* K, Nemes-Vetéssy* Zs, Burger* K; Extended NMR study of spin-crossover compounds [Fe(1-alkyl-1H-tetrazole)$_6$]$(BF_4)_2$ and their Zn^{II} analogs; *Structural Chemistry;* **14**, 349-368, 2003

H.4. Mitroova* Z, Zentko* A, Trpcevska* J, Lukacova* M, Csach* K, Bokor M; Rare earth ferricyanides; *Diffus Defect Data B;* **90-91**, 85-90, 2003

H.5. Péter L, Almási* B, Verő* B, Schneider* H; Theoretical analysis of entrapment kinetics in hydrogen permeation experiments; *Mater Sci Eng A;* **339**, 245-254, 2003

H.6. Péter L, Almási* B, Verő* B, Schneider* H; Theoretical analysis of hydrogen permeation and entrapment kinetics; *Materials Science Forum;* **414-415**, 305-310, 2003

H.7 Péter L, Szűcs* E, Filák* L, Verő* B, Schneider* H; Electrochemical hydrogen permeation on steel sheets with in situ electrodeposition of a Pd layer at the exit side; *J Appl Electrochem;* **33**, 613-617, 2003

H.8. Tompa K, Bánki P, Bokor M, Lasanda G, Vasáros L*; Diffusible and residual hydrogen in amorphous Ni(Cu)-Zr-H alloys; *J All Comp;* 3**50**, 52-55, 2003

H.9. Weihnacht* V**,** Péter L, Tóth J, Pádár J, Kerner* Zs, Schneider* CM, Bakonyi I; Giant magnetoresistance in Co-Cu/Cu multilayers prepared by various electrodeposition control modes; *J Electrochem Soc;* **150**, C506-C515, 2003

H.10. Zentko* A, Bokor M, Lukacova* M, Marysko* M, Mihalik* M, Mitroova* Z, Zentkova* M; Magnetic properties of Pr[Fe(CN)6]·5H_2O; *phys stat sol (a);* **196**, 340-343, 2003

H.11. Bakonyi I, Tóth J, Kiss LF, Tóth-Kádár E, Péter L, Dinia* A; Origin of GMR contributions in electrodeposited Ni-Cu/Cu multilayers; *J Magn Magn Mater;* accepted for publication

H.12. Meuleman* WRA, Roy* S, Péter L, Bakonyi I; Effect of current and potential waveforms on GMR characteristics of electrodeposited Ni(Cu)/Cu multilayers; *J Electrochem Soc;* accepted for publication

H.13. Péter L, Liu QX, Kerner Zs, Bakonyi I; Relevance of potentiodynamic method in parameter selection for pulse-plating of Co-Cu/Cu multilayers; *Electrochim Acta;* accepted for publication

See also: I.3., I.4., I.7., J.11., O.12.

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, G. Rischák, F.I. Tóth, I. Varga

Soft magnetic nanocrystalline alloys. — A new family of cast iron-phosphorus based bulk amorphous alloys have been developed and prepared in rod forms up to 3 mm diameter by centrifugal casting. A new family of Nanoperm alloy was developed based on phosphorus instead of boron. We are continuously searching for the optimal composition. The new high-temperature Co-based nanocrystalline alloy ($Fe_{85-x}Co_xNb_5B_8P_2$) which was developed in the previous year and can be cast in air has been studied thoroughly within the EU project. The simulation of superparamagnetic magnetization curves was solved successfully by the Genetic Algorithm method in order to extract the distribution of the magnetic moments. In this way, a so-called Langevin granulometry method was established and applied for nanocomposites. The critical size for monodomain particles has been studied by micromagnetic simulations and a series of transitional states have been discovered from mono-to-multidomain states, depending on the composition. This result is important in interpreting the Langevin granulometry results and to convert the magnetic moment distributions into particle size distributions. A new tester has been built for measuring the power loss at high frequencies (between 100 kHz and 600 kHz). A switch-mode power supply for telecomunnication applications has been developed, by using only nanocrystalline alloys as inductive elements. This work was centered around the tasks of our ressearch grants OTKA T-034666: ”Bulk amorphous alloys”, NATO Science for Piece program (Nr. 971930): “Magnetic Nanocomposites” and EU grant CRD2-2000-30349: “Soft magnetic nanomaterials for high temperature and high frequency functional applications in power electronics”.

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Grants and internationa cooperations

OTKA T-034 666 Iron-based bulk amorphous alloys and nanocomposites (L.K. Varga, 2001-2004)

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[+] Permanent position: Loránd Eötvös University, Budapest

OTKA T-035 278 Correlation between domain structure, dynamical magnetic properties and structural factors in soft magnetic equilibrium and metastable alloys. (Research grant of the Budapest University of Technology and Economics, participant: P. Kamasa, 2001-2004)

OTKA T-037643 Nanostructured functional coatings. (Research grant for the Chemical Research Center of HAS, participant: L.K. Varga, 2002-2005)

NATO Science for Peace Project 971930: Magnetic nanocomposites for transformer cores and magnetic refrigeration (L.K. Varga, 1999-2003)

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

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

NKFP-3A/0050/2002 Széchenyi NRP: Development of nanostructured coatings with unique properties by using environmental friendly methods (Participant: 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, 2001-2003, Hungarian-French Bilateral Science and Technology Cooperation)

HAS-SAS Study of physical properties of special magnetic materials (L.K. Varga, 2001-2003, Hungarian-Slovakian Academy Exchange Programme)

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

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See also H.1., H.9., J.35., O.8

J. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

L. Rosta, L. Almásy, L. Cser, , I. Füzesy, J. Füzi, A. Len[#], M. Markó[#], Á. Nagy, E. Rétfalvi[#], L. Riecsánszky, Zs. Sánta[#], N.K. Székely[#], 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 for basic and applied research, commercial utilisation and education. Experiments were completed in 2003 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 neutron scattering (SANS) instrument, a reflectometer (REFL), a triple axis spectrometer (TAS) and a cold neutron test facility. 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 Los Alamos National Laboratory, HMI Berlin or LLB Saclay (France).

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.

Neutron optics. — Atomic resolution neutron holography constitutes a novel technique to obtain structural information. It is based on the recording of the interference of neutron waves coherently scattered by atoms located on a crystal lattice with a suitable reference wave. The experimental realization of neutron holography studies has been continued. We have proposed, that atomic resolution holography can be achieved by two ways. The inside source concept uses nuclei possessing 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 second series of experiments we used the inside source concept to image Pd nuclei in a single crystal. This process can be accomplished by two complementary schemes. In the frame of this approach, a point-like source of spherical neutron waves is required inside a single crystal. Such a source can be realized owing to the extremely large value of the incoherent neutron scattering cross section of the proton. The interference between the undisturbed wave field and that part of the wave which is scattered by neighboring atoms can be recorded, thereby producing a hologram. The experimental feasibility of this internal source method was proven by us on a $PdH_{0.8}$ single crystal.

Liquids. — Aqueous solutions of some alcohols with two or three hydroxyl groups were studied by small-angle neutron scattering. Many of these polyols exhibit tendency to aggregate depending on the size of the alkyl chain and the positions of the hydrophilic OH groups. The aim of this project is to explore the mechanism of the hydrophobic interaction for these systems, which is the main governing factor of the aggregation of water-soluble molecules having hydrophobic parts. Small-angle scattering allows one to see the structure of the formed aggregates with moderate resolution, as well as to quantify the degree of self-association of the components. This latter parameter can be used to correlate the degree of aggregation of different series of diols with the positions of the OH groups. Until now only

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three systems have been studied, so there is not enough data for such comparison. Analyses of the form of the aggregates in these solutions led to conclusion that the aggregated diols do not form micelles, but form rather loose structures, resembling statistical concentration fluctuations.

Industrial application. — Small angle neutron scattering (SANS) technique has been used to study the microstructural evolution of precipitates in real pistons of racing cars made from commonly used AlSi2CuNiMg alloy. The experiment was performed on new and worn out piston crowns. The SANS curves were measured in 5 different points (possible critical locations) of both pistons. The inserts in Fig.1. show the investigated points and the 2D scattering images. On the central points of the new (unused) sample we have observed isotropic scattering, but on the lateral parts of the piston the scattering became anisotropic indicating presence of texture induced by manufacturing. The Al-Mg-Si alloys exhibit mechanical properties, which are highly sensitive to thermal treatments. The operating temperature is usually very close or, in certain parts of the crown, can exceed the ageing temperature. We compared the alteration of mechanical properties caused by the ageing treatment with the changes of size distribution of precipitates.

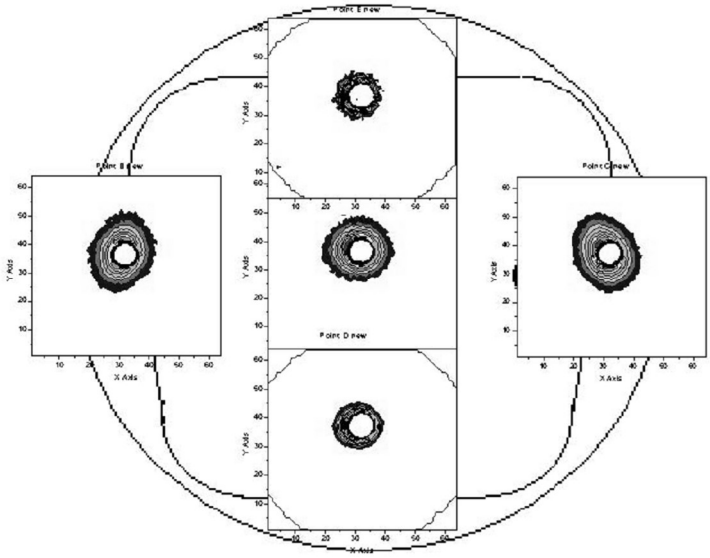

Fig.1. Investigated points in the pistons and the 2D scattering images

Instrumentation development. — Hexapole neutron lenses approximating the Halbach structure using brick-shaped NdFeB permanent magnets have been realized with aperture diameter 7 mm, achieving two thirds of the ideal field strength. The neutron optical characteristics have been tested in neutron beam experiments, using a 2D position sensitive detector in time-of-flight regime (Fig.2.). The hexapole field constant 47000 T/mm^2 has been proven by both magnetic and neutron beam measurements.

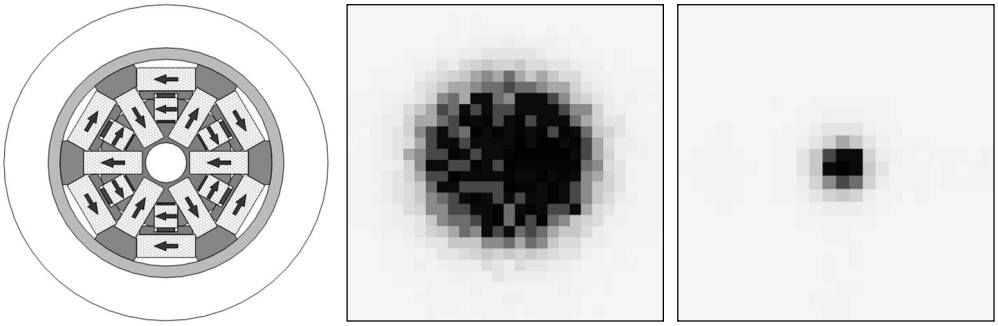

Fig.2. Hexapole lens structure, beam without lens and focussed beam

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Grants and international cooperations

EU ERB PL96-9007 Neutron Round Table (L. Rosta, 2001-2004)
ICA1-CT-2000-70029Centre of Excellence (CMRC, WP1, 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, 2000-2003)

OMFB 01582/02	Research & development of neutron optical devices (L. Rosta, 2002-04)
OMFB 01718/02	Development of particle beam chopper system (L. Rosta, 2002-04)
OMFB-00367/02	Magnetic neutron optical devices (L. Rosta, 2002-03)
OTKA T 22486	Investigation of sintering processes (P. Harmat, MFA, participant: E. Rétfalvi, 1999-2003)
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, senior scientist, St.Petersburg Nuclear Physics Institute, Russia, August 10 – September 10 (host: Gy. Török)

— Cs. Muzsnay, Professor, University Sapientia, Romania, July 10-August 10 (host: L. Almásy)

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K. NEUTRON SCATTERING

E. Sváb, M. Fábián[#], I. Harsányi[#], L. Kőszegi, Gy. Mészáros, L. Pusztai, Z. Somogyvári[#], L. Temleitner[#]

Amorphous systems. — The structure of (vapour deposited) **amorphous silicon** (a-Si) have been considered by Reverse Monte Carlo (RMC) modelling, based on neutron diffraction data. It was pointed out that the existence of small bond angles of the order of about 75 degrees are necessary for describing the experimental structure factor correctly. These small bond angles, in turn, result in higher energy states in the gap region of the electronic density of states. These higher energy states were found to be localised on atoms involved in forming the small bond angles. Such local atomic arrangements have been proposed as a new type of defects in evaporated a-Si.

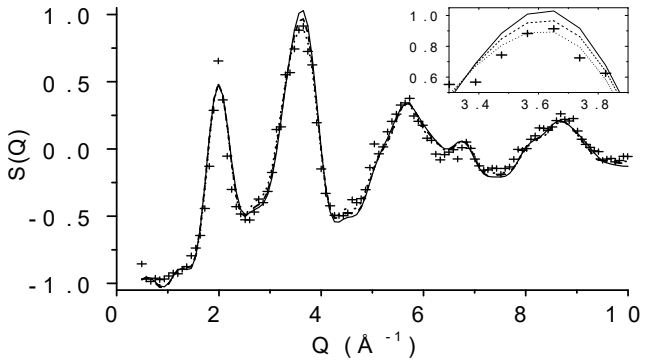

Figure 1. Total structure factors of amorphous silicon. Symbols: neutron diffraction data; solid line: RMC model after 100000 accepted moves; dashed line: RMC model after 250000 moves; dotted line: RMC model after 500000 accepted moves. Note that this last model describes experimental data the best (see insert).

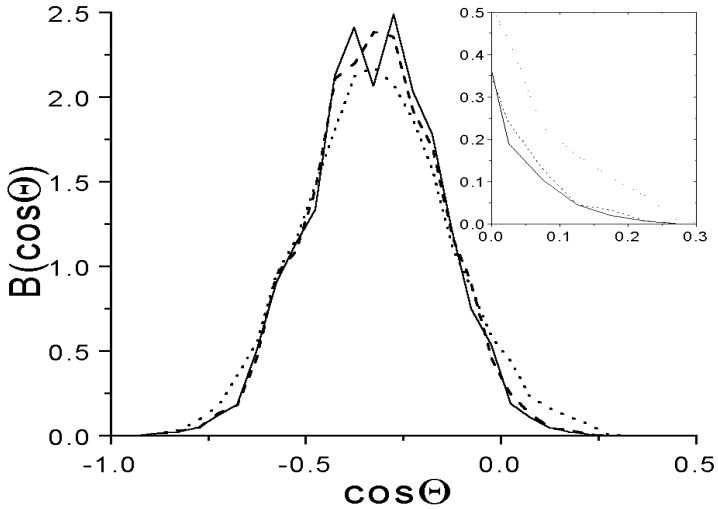

Figure 2. Cosine distribution of bond angles for the three RMC model shown in Figure 1 (notation is the same). Note that the model that best fits experimental data has the greatest number of small bond angles.

[#] Ph.D. student

Borosilicate glasses are of significant current interest as suitable materials for isolating host media for radioactive waste materials. Neutron diffraction study has been undertaken on a series of samples with a general formula of $(65\text{-}x)SiO_2{}^*25\ Na_2O{}^*5BaO{}^*5B_2O_3{}^*xZrO_2$ ($0 \le x \le 5$). Despite the great hydrolytic stability of the samples, the first few experiments revealed their tendency to superficially adsorb H_2O. In order to obtain information on the local structure of this multicomponent system, RMC simulation was applied. The final RMC fit matched fairly well the experimental structure factors. Most of the partial pair-correlation functions of the glass network has been calculated directly from the structural model.

Liquids. — The structure factor of a hydrogen (^1H) containing material, liquid **bromoform**, CBr_3H was determined. For the correction of the sloping background, due to the incoherent scattering from ^1H, a novel procedure was applied which is embedded in the RMC modelling algorithm. Some of the partial pair correlation functions of CBr_3H has been calculated from the RMC model; comparison of the C-C and Br-Br partials with equivalent functions of the deuterated compound, CBr_3D, shows fair agreement.

The static dielectric constant (ε_0) of **ambient liquid water** was calculated from RMC models of the material, on the basis of the Kirkwood-Fröhlich theory. For the purpose, RMC simulations with over 200 million accepted steps were performed. Large fluctuations in the individual ε_0 values have been found even for quite large system sizes. As a corollary, it was found that the pathologically high dipole moment of the water molecules in systems where earlier partial pair correlations functions have been fitted by RMC is caused by the - unphysical - large distortion of the H-H intramolecular distance.

Manganites. — Bi-based manganites $Bi_{1-x}A_xMnO_3$ (A=divalent alkaline cation) have attracted interest due to the significantly higher temperatures of charge ordering as compared to their perovskite-like counterparts $R_{1-x}A_xMnO_3$ (R=rare earth). We undertook a neutron powder diffraction study on $Bi_{0.25}Ho_{0.25}Ca_{0.5}MnO_3$ and $Bi_{0.5}Ca_{0.5}MnO_3$ at 10 K and at room temperature. Our main goal was to specify the role of $\langle r_A \rangle$ in the structural distortions, potential charge ordering and magnetic ordering phenomena. At room temperature, the diffraction pattern has revealed that $Bi_{0.25}Ho_{0.25}Ca_{0.5}MnO_3$ is in paramagnetic phase of small monoclinic distortion, allowing for structural description in orthorhombic Pnma symmetry. At 10 K a charge-exchange type antiferromagnetic phase was established, which is characteristic of the insulating Mn^{3+}/Mn^{4+} charge-ordered state. At low temperature, a superstructure developed that was successfully modelled in monoclinic symmetry, refined in space group $P2_1/m$.

Neutron depolarisation. — Finemet ($Fe_{73.5}Si_{13.5}B_9Nb_3Cu_1$) is an extensively studied material because of its great technical importance. Below the Curie temperature of the amorphous phase the magnetic interaction between the nanoparticles results in excellent soft magnetic properties. We have performed three-dimensional neutron depolarization investigations to study the bulk domain structure as a function of external magnetic field (0-24 A/cm) and temperature (300-623 K), both on stress-annealed and standard heat-treated materials. It was established that during annealing a hard magnetic axis parallel to the stress direction develops. Although the shape of the material suggests a magnetization distribution inside the plane of the ribbon, our results clearly show that plane magnetization components perpendicular to the ribbon surface also exist. This statement is evidenced by the reduction of the D_{zz} component of the depolarization matrix. For the case only z-domains exist, the neutrons, initially polarized in the z-direction, would not interact with the magnetization of the sample, thus D_{zz} should be 1. A model has been developed to interpret this remarkable result.

Radiography. — In order to inspect possible defects in the composite structure of **helicopter rotor blades**, combined neutron- and X-ray radiography measurements have been performed and analysed. The rotor blades are about 10 m long, therefore the radiography images are taken in several well-adjusted segments, and a special software program has been developed to reconstruct the whole radiography image. Imperfections in the honeycomb structure, resin rich or starved areas at the core-honeycomb surfaces, inhomogeneities at the adhesive filling and water percolation at the sealing interfaces of the honeycomb sections have been revealed by neutrons (Fig.3.). The localization of structural metal parts were analysed by X-ray radiography.

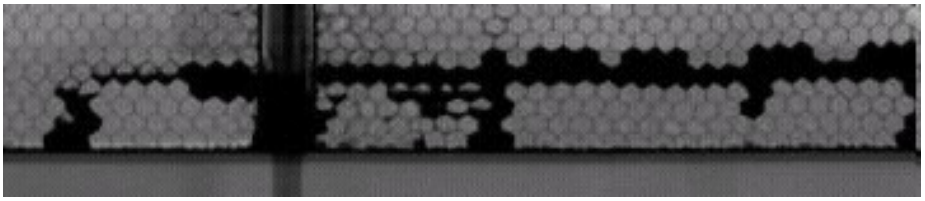

Fig.3. Honeycomb structure of a helicopter rotor blade section (90×30 cm2) with an extensive water percolation (dark areas) as revealed by neutron radiography

Internal stress. — Quenched-in internal stresses have been measured on precipitated Cu grains in **FeCu(5%) alloy** as a function of quenching temperature. Elastic stresses were determined from the (111) peak shift, while changes in the peak broadening may be connected to the plastic stresses or to the access precipitations that gradually appear below the solubility limit of Cu in Fe. During the homogenising treatment (850 °C, 3h) only the Cu amount above the solubility limit precipitates on the grain boundaries of the Fe grains. At lower temperature, more Cu precipitates, but only within the grains. These two processes are responsible for the peculiarities of the broadening.

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Grants and international cooperations

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

OTKA T 042495 Neutron diffraction study of atomic and magnetic structures (E. Sváb, 2003-2006)

EU HPRI-CT-1999-50013 Software for computer Aided Neutron Scattering (L. Pusztai, 2000-2003)

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

OMFB-00012/2003 Structure studies with neutrons at the Budapest research reactor (E. Sváb, 2003)

Bilateral travel grant of the Hungarian and Bulgarian Academies of Sciences, No. 5. Structure studies by neutron diffraction (E. Sváb, 2000-2003)

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 as a post-doctoral fellow for 2 years starting at 01.01.2002 (Host: L. Pusztai).

— Margit Fábián (student), Babes-Bolyai University, Romania; 1 April- 30 May 2003 (Host: E. Sváb)

— Rodica Sinka (student), Babes-Bolyai University, Romania; 1 April- 30 May 2003 (Host: E. Sváb)

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See also E.7.

L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, S. Varró

Experimental research. — Recent superintense ultrashort laser pulses with femtosecond pulse envelope may contain few, only 1-2 electromagnetic cycle oscillations. The phase difference between the maximum-value electromagnetic cycle amplitude and the pulse envelope-maximum (called "absolute phase") is strongly varying in the course of propagation through any dielectric material (including laser elements). This phenomenon strongly affects the (nonlinear) interaction of superintense few-cycle pulses with matter.

Using the multiphoton (and tunnel) electron emission from a metal surface discovered by us earlier as a nonlinear interaction process, we have participated in the experimental determination of the absolute phase of a 5 femtosecond duration (2 cycle) laser pulse emitted by a Titanium:Sapphire laser. Inversely, in possession of the measured changes of the absolute phase, its minimalization and stabilization may be realized by feedback to the laser performance. These works have been performed in cooperation with the Austrian group at the Technische Universität in Vienna.

Theoretical research. — On the basis of the Hamiltonian form of the Klein-Gordon equation for a charged scalar particle field introduced by Fehbach and Villars, the gauge-invariant 2×2 Wigner matrix has been constructed whose diagonal elements describe positive and negative charge densities and whose off-diagonal elements correspond to cross-densities in phase space. The system of coupled transport equations (Quantum Boltzmann-Vlasov Equations) has been derived in the case of interaction with an arbitrary external electromagnetic field. A gauge-independent generalization of the so–called free-particle-representation due to Feshbach and Villars has been given, and on the basis of it both the nonrelativistic limit and the classical limit of the Quantum Boltzmann-Vlasov Equation have been discussed. In the nonrelativistic limit ($p/mc \to 0$) the set of equation of motion decouples to two independent quantum transport equations describing the dynamics of oppositely charged positon and negaton densities. In the classical relativistic limit ($h \to 0$) two relativistic Boltzman-Vlasov equations result in the diagonal positon and negaton densities. Even though the Planck constant h is absent from the latter equations, the real part of the positon-negaton cross-density does not vanish.

By using merely classical electrodynamics the reflection and transmission of a few-cycle femtosecond Ti:Sa laser pulse impinging on a thin metal layer have been analysed. The thickness of the layer was assumed to be much smaller than the skin depth of the radiation field, and the metallic electrons were represented by a surface current density. The interaction of the electrons with a periodic lattice potential has also been taken into account. The presence of this nonlinear potential leads to the appearance of higher harmonics in the scattered spectra. A formal exact solution has been given for the system of the coupled Maxwell-Lorentz equations describing the dynamics of the surface current and the radiation field. Besides, an analytic solution was found in the strong field approximation for the Fourier components of the reflected and transmitted radiation. In our analysis particular attention has been paid to the role of the carrier-envelope phase difference of the incoming few-cycle laser pulse. The interaction of a few-cycle femtosecond laser pulse with a surface current is analysed. It has been shown that the high-harmonic spectra of the scattered waves strongly depend on the carrier-envelope phase difference.

For some time now anomalous transparency induced by high intensity laser light interacting with thin solid foils has been found experimentally. In our study based mostly on classical electrodynamics the increase of transmittivity is the consequence of the more and more pronounced role of the frustrated total reflection in the plasma layer. We have given a detailed analysis of the effect of electron temperature and of the angle of incidence of the laser light on the transmittivity of the strong laser pulse.

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Grants and international cooperations

OTKA T032375 Experimental and theoretical investigation of fundamental laws related to laser-matter interactions of intense field QED, based on the latest achievements of laser physics. (Gy. Farkas, 2000-2003)

TéT–A-1/01 Hungarian-Austrian Bilateral Scientific and Technological Cooperation, Subject of research : Interaction of electromagnetic radiation with matter on an ultrashort time scale (S. Varró, 2002-2003)

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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M. LASER PHYSICS

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

Hollow cathode lasers. — Ultraviolet hollow-cathode metal ion lasers can be used as light sources for UV Raman and laser-induced fluorescent spectroscopy. These lasers are usually excited by charge transfer reactions between noble gas ions and metal atoms. High density of noble gas ions are created in hollow-cathode discharges while the necessary metal atom density can be produced either by thermal evaporation or utilizing the cathode sputtering effect of the discharges. High-voltage hollow-cathode arrangements have been developed during the last ten-years period to increase the efficiency of sputtered lasers. Our recent investigation is focused on the development of a 224 nm segmented hollow-cathode silver ion laser. Our aim is to prolong the lifetime of the laser tube in order to meet the requirements of commercial production.

Gas discharge and plasma research. — We investigated the light emission from glow discharges, with special attention to the radial distribution profiles. The results of self-consistent computer simulations showed a good agreement with earlier experimental data. The effects of heavy-particle processes (fast ion - atom and fast atom - atom collisions) on the operation of high-voltage (1000 V $\leq V \leq$ 5000 V) glow discharges were also analyzed through computer simulations. In the field of strongly coupled plasmas we have studied the spatial-temporal localization of particles in liquid-phase strongly-coupled plasmas. 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. We have also determined the Einstein frequency spectra of particle oscillation in the liquid phase of strongly coupled Coulomb and Yukawa systems. We have thoroughly investigated the dynamical properties of layered systems of charged particles by molecular dynamics simulations, through computations of the correlation spectra of fluctuations of mass density, as well as of longitudinal and transverse currents, which also yield the dispersion characteristics of the systems.

Electrolyte cathode atmospheric pressure glow discharge. — A special arrangement was developed, in which the electrolyte flows through a narrow capillary glass tube. In this way an abnormal type glow discharge was produced in which a significant enhancement of the current density, the cathode fall and the intensity of metals dissolved in the solution could be observed compared with our earlier experiments. To clarify the basic properties of this capillary discharge, a special optical system was used to investigate the vertical distribution of the gas and the electron temperature and also the metal line intensities using spectroscopic methods. The gas temperature was determined from the rotational temperature of the OH band: the intensity ratio of the OH 306.776 nm and the OH 308.986 nm band lines were measured. The obtained experimental results agree with our earlier data obtained by calculations taking into account the different gas discharge processes. Since the discharge uses an electrolyte cathode, the discharge operates in saturated water vapour. In spite of this, a significant intensity of the N_2 – 337 nm band could be observed, which probably originates from the outer edge of the discharge plasma.

Ellipsometry. — We have successfully finished the development of a new multispectral imaging ellipsometer system. The new technique uses divergent illumination from a point-like light-source and after reflection from the target, the automatically projected image of

[#] Ph.D. student

the sample is acquired on a CCD-camera giving multiple angle-of-incidence and polarization state mapping information. A fiber-coupled “Tricolor” laser system enables us to proceed the real time quality control of large (up to 5”) semiconductor surfaces.

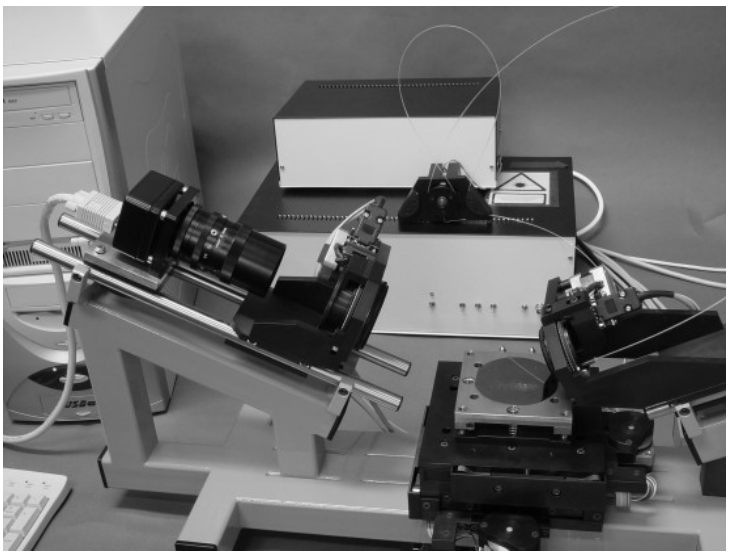

Fig 1. Imaging multispectral ellipsometer

Spectroscopy. — The role of the *Stark effect* in the mode properties of a He-Cd^+ laser excited in a hollow cathode discharge was analysed. It was found that – in this laser – Stark broadening can give a significant contribution to the homogeneous line-broadening; it depends, however, on the properties of the atomic levels involved. Actually it was shown that for the green He-Cd^+ laser the increased homogeneous line-width results in single mode operation, while for the blue one it does not, as it was experimentally observed earlier.

In order to explain the properties of the *optogalvanic effect* (OGE) occurring at the 667.7 nm Ar line in a hollow cathode discharge a model was developed. The model is based on various excitation processes and radiation trapping between the Ar ground state and first excited states is taken into consideration. On the basis of the model the excitation path leading to the OGE was clarified and the measured change of the optogalvanic signal amplitude and sign along the cross-section of the discharge tube could be explained.

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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 - 34156 Modern plasma simulation techniques (Z. Donkó, 2001-2004)
MTA-OTKA-NSF 28 Strongly coupled Coulomb systems (Z. Donkó, 2001-2003)
OTKA T-042493 The role of ions of the basic electrolyte solution in the electrolytic cathode atmospheric pressure glow discharge (P. Mezei , 2003-2006)
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N. METAL OPTICS

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

A new type of PSTM (plasmon scanning tunneling microscope) was constructed and recently tested cooperating with the STM group of the Max Planck Institute for Quantum Optics in Munich (Germany). 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, ii) the thermal behaviour (Seebeck potential and thermal dilatation) and, iii) of course the tunnel current proportional to the surface roughness. As usual, the thermal signal has the largest time constant, i.e. its rise time is the slowest.

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 conventional topographic picture (ch.1) is made simultaneously with the plasmon (ch.2) and thermal (ch.3) pictures.

In order to estimate experimentally the plasmon and thermal components of the detected images, measurements were made on 49 nm thick gold metal films laser ablated with silver using 2 J energy pulses of a Nd:glass laser in $1x10^{-3}$ Pa vacuum and a massive silver target. The resulted overlayer was 0.8-1.6 nm thick, in average. 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. A gold tip was used for the measurements, because its response for the silver is higher than for other metals.

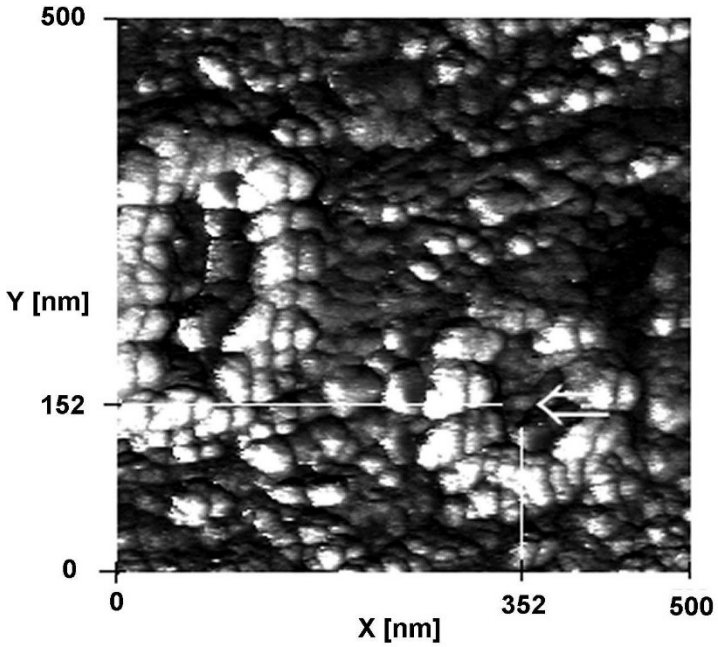

Fig.1. Craters formed in a 49 nm thick gold layer by laser sputtering of silver. Average silver thickness: 1.6 nm. (An AFM image.) Arrows show the partly buried silver cluster.

A mathemathical analysis was made on the plasmon images observed on 50 nm thick gold and silver layers. The FFT (fast Fourier transformation) diagrams show multiple frequency surface plasmon Fourier components. This means that, evidently, nonlinear plasmon scattering on the roughness of metal surface induced coherent scattering, interference and frequency multiplication.

Further testings of the instrument and other measurements studying the near-field optics are in progress.

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Grants and international cooperations

OM 00224/2001 Széchenyi NRP "Nanotechnology" (2001-2003)

Max Planck Institute for Quantum Optics (Garching, Germany): Surface plasmon research using STM.

Physical Institute of University of Bonn (Germany): Charge density waves in photorefractive materials.

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N.2. Kroó N, Szentirmay Zs; Quantum properties of surface plasma oscillations on metallic surfaces?; *CEJP*; accepted for publication

Conference Proceeding in Hungarian

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O. LASER APPLICATION

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

Optical measuring techniques. — Based on a new dual wavelength forward-backward scattering laser particle measuring method, a new instrument 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. In the instrument we used two different lasers (green and red), four detectors (forward and backward scattering for both wavelengths), special electronic filtering and data evaluation.

In the frame of NRDP ***Atmospheric Pollution of the Atmosphere,*** a mobile laboratory for environmental monitoring of atmospheric aerosols and measurement of air contamination installed in a FIAT DUCATO microbus was equipped by new instruments – KS304 sampler, KS 308 cascade impactor, Metler Toledo scale, etc. The laboratory participated in two measurement campaigns in the summer and autumn of 2003. The results of different measurement methods (gravimetric, light scattering, impaction) for determination of the air contamination were compared and analyzed.

In the frame of the NRDP **Nanotechnology** project measurement automatization was carried out in the *VELOSIZER* measurement setup. The system is constucted for the simultaneous measurement of the size and velocity of nanometer scale particles. In this respect a computer controlled goniometer with 10 arc second resolution and a computer controlled two axes X-Y position transducer with 0.3 μm resolution was incorporated in the measurement system.

Fig 1. Inteligent Laser Warner System installed on the vehicle

In the frame of the program of the Ministry of Defense the development of the Inteligent Laser Warner System was finished. The system is installed on one of the armoured vehicles of the Army (see Fig.1.). The system works on the early warning and measurement of direction of propagation of laser range finder impulses. Military testing is currently in progress.

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 stabilized semiconductor lasers, fiber optical light guides and avalanche photodiodes is currently under performance for the purpose of system optimization.

In the frame of this project a high resolution interferometric surface testing system was developed. A frequency stabilized He-Ne laser, a high quality optics and a new data evaluation method enables the scanning of surfaces with sub-nano resolution.

[#] Ph.D. student

Development of measurement techniques based on statistical properties of scattered light on ensemble of aerosol particles is in progress. Numerical simulation of scattering statistics on ensemble of aerosol particles was performed.

A quantum-optical measurement system for the standardles determination of the quantum efficiency of the photon counting detectors using entangled photon pairs was finished.

The principle of a new pre-determined photon number light source was proposed. The laboratory experimental setup for such new light source was constructed. Main parameters of the system have been calculated.

Amorphous carbon layers. — Soft amorphous carbon layers exhibit intensive light emission in a wide photon energy range, including even ultraviolet photons. Development of photodiodes and sensors with amorphous carbon as an active layer is quite reasonable, and requires luminescence quantum efficiency enhancement, or an increase of the amount of emitted light from the carbon films. Therefore a comparative study of luminescence efficiency as well as the emission spectral range have been performed on amorphous carbon samples, prepared by different deposition technique and process parameter values. Resonant enhancement of light intensity at given wavelengths was also investigated. A detailed examination of the luminescence excitation spectra by measuring 3D emission excitation curves provided a valuable method to control electronic levels important in luminescence process.

Surface Enhanced Raman Scattering (SERS) technique was introduced to study amorphous carbon films. The technique is well elaborated for liquid sample investigation; we worked out the study of solid carbons by this method. The crucial problem in this case is to prepare carbon-free enhancing agent, the silver colloid. We were successful in preparing the colloid by sodium hydro-borate, containing no carbon. Few orders of magnitude enhancement was archived in Raman cross section. Sometimes intensive fluctuations appeared, like what can be seen on Fig. 2. These fluctuations show very unusual pattern both in frequency and time. The features of these processes might provide possibility to enhance the resolution of the Raman scattering.

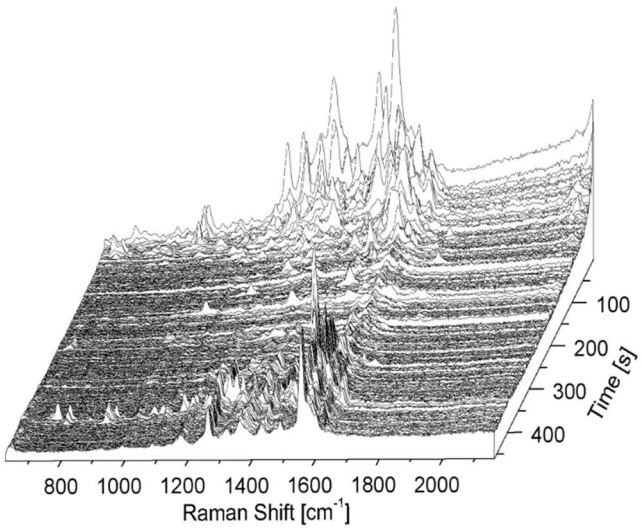

Fig. 2. A time series of fluctuating SERS spectra detected on the sheet surface of HOPG.

The Raman spectrum of most graphitic amorphous materials contains, beside the graphitic (Graphitic, G and Disorder-related D) peaks, two others in the region of the well studied two peaks of poly-acetylene. We have concluded that these vibrations originate probably from the edge region of the graphitic sheets.

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Grants and international cooperations

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

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

Hungarian-Greek Intergovernmental S & T Cooperation Programme GR-31 (I. Pócsik, 2002-2003)

Hungarian-Ukrainian Intergovernmental S & T Cooperation Programme UK-6, (I. Pócsik 2003-2004)

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

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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 P.1.

P. FEMTOSECOND LASERS

R. Szipőcs, Á. Bányász[#], A. Lukács[#]

Optical thin-films in femtosecond laser systems. — Continuing our research which 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 for a mirror dispersion controlled, tunable, 100 fs Ti:sapphire laser mode-locked by a semiconductor saturable absorber mirror built in our laboratory and (b) low reflection loss multicavity Gires-Tournois mirrors for our femtosecond pulse infrared optical parametric oscillator (IR OPO) in collaboration with R&D Ultrafast Lasers Ltd., Hungary, and MLD Technologies, USA. The former MCGTI mirrors exhibit reflectivities R > 99.97% and negative group delay dispersion of –90..-110 fs^2 over a bandwidth of 780 to 880 nm, while the MCGTI mirrors developed for the IR OPO has a special design that allows us depositing the dichroic mirror shown in Fig. 1 (left) and the negative dispersion mirror shown in Fig. 1 (right) during a single coating run. Both designs exhibit low reflection loss relative to previous designs based on the chirped mirror design concept, which allowed us building diode pumped fs oscillators using pump powers as low as a few hundred mW-s and IR OPO-s with increased output powers.

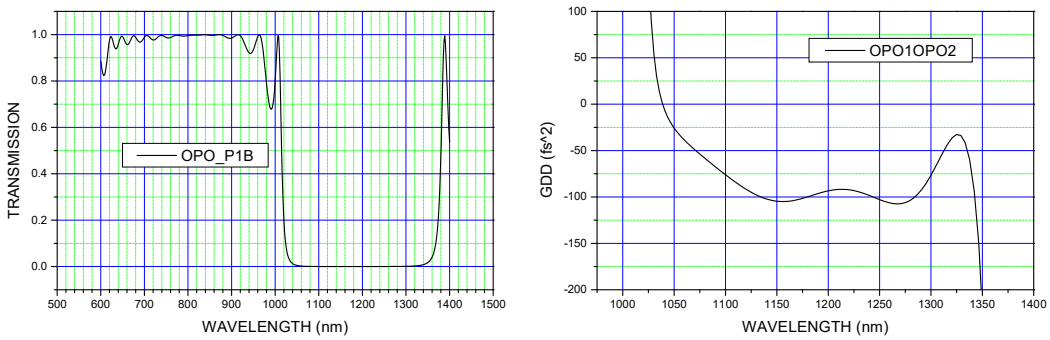

Fig. 1 Transmittance (left) and group-delay dispersion (GDD) of the dielectric mirrors developed for an IR OPO

Pulse compression in microstructure (photonic crystal) optical fibers. — In collaboration with OFS Fitel Laboratory (USA) and R&D Ultrafast Lasers Ltd., 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 these 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. 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. We are convinced that our proposed simple "upgrade" for 100 fs pulse laser

[#] Ph.D. student

oscillators will help to reduce considerably the temporal resolution of ultrafast measurements in many ultrafast spectroscopy laboratories.

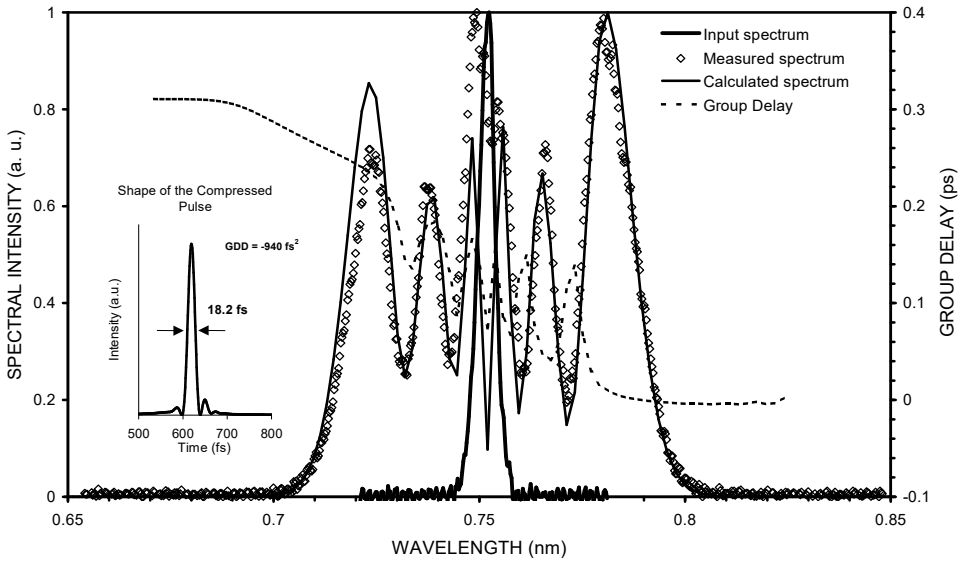

Fig.2 150 fs to 18 fs pulse compression by a microstructure optical fiber and dispersion compensation

In collaboration with researchers at the University of Pecs, Hungary, we performed z-scan measurements on $LiNbO_3$ samples of different doping concentrations and compositions in order to determine their optimal composition for nonlinear frequency conversion by periodically poled $LiNbO_3$ (PPLN). The result of such a measurement is shown in Fig. 3.

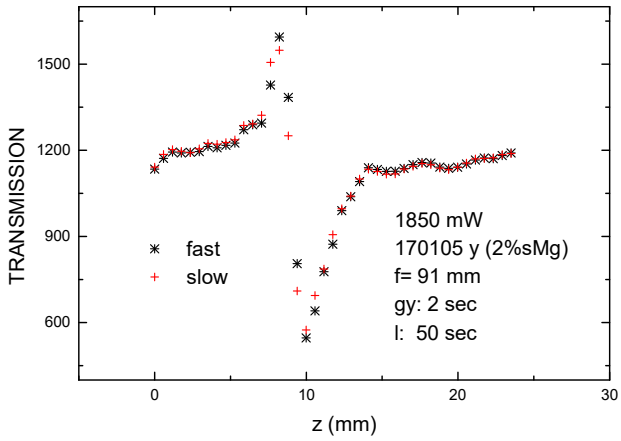

Fig. 3 The result of a z-scan measurement on a $LiNbO_3$ sample (sample No. 170105, 2% Mg doping)

In our fs pulse IR OPO, the KTP crystal used for nonlinear frequency conversion has been replaced by a PPLN sample, which resulted in an increased conversion efficiency. Another advantegous feature of this latter concept is that the IR OPO can be independently tuned from the fs pulse pump (Ti:sapphire) oscillator by changing the grating period of the PPLN crystal, which allows independent tuning of the (frequency doubled) pump and probe pulses in our femtosecond time resolved specroscopic measurements on different dye samples.

In collaboration with R&D Ultrafast Lasers Kft., Budapest, and with the Laser Physics Laboratory of Synchrotron Trieste, Italy, a tunable, 100 fs, mirror dispersion controlled Ti:sapphire oscillator was developed in which mode-locking was achieved by the use of semiconductor saturable absorber Bragg reflector. The laser can be operated in the 800-860 nm regime without the need of any adjustment of the cavity elements but the Lyot filter tuning element. The tuning range of the laser is currently limited by the reflectance band of our saturable absorber mirror.

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Grants and international cooperations

NKFP3-00164/2001 Széchenyi NRP: Nanotechnology (Coordinator: J. Gyulai, MFA, participant: R. Szipőcs, 2001-2004)

Publications

Article

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See also R.19.

Q. OPTICAL THIN FILMS

K. Ferencz

Optical thin film structures consisting of nanoscale laminated layers. — We have continued our research concerning the development of optical thin film structures containing 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, hafnia, aluminium and silver layers. Using needle-like optimization thin film design method, we have succesfully produced many kinds of ultrafast nanooptical coating systems - octave-wide-band, low dispersion antireflection coatings, low dispersion beamsplitter coatings, low dispersion protected silver-mirrors, ultrafast dichroic mirrors and harmonic separators, output coupler mirrors, Gauss-filters for amplifiers, for example. Our newest polarizing beamsplitter cubes has better than 2000 : 1 extinction ratio, if the prism material is BK7 optical glass, the high-index material is TiO_2, the low-index material is SiO_2, at laser wavelengths between 505 and 550 nm.

Other developments on optical coatings. — Our work on ultrafast optical coatings is still in progress cooperating 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 succesfully developed new type of ultrawideband antireflection coatings for tilted-front-interface chirped mirror devices, for the reduction of the fluctuations of the group delay dispersion of the conventional dispersive mirrors, which opened 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 nonlinear optical material. Using our microstructured coating samples new types of biologically active nanotechnological devices are researched in cooperation with the Biophysics Institute at the Szeged Biological Research Centre (Prof. Pál Ormos). Our work on interference filters is still in progress for high sensitivity detection of protein molecules elaborated by gene manipulation methods.

These results were obtained in the frame of the scientific cooperation between 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, 2000-2003)

NATO SfP 974262 Optoelectronic Devices Based on the Protein Bacteriorhodopsin (Coordinator: C.E. Wolf, Deutschland, participant: K. Ferencz, 2000-2005)

NKFP3/064/2001 Széchenyi NRP: Nanotechnology (Coordinator: J. Gyulai, MFA, 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, 2001-2004)

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

NKFP1A/0010/2002 Research and development of PET minicamera devices (Coordinator: L. Trón, Ped. Centre, Debrecen, participant: K. Ferencz, 2002-2007)

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. — The absolute values of the effective non-linear coefficients (d_{eff}) of $CsLiB_6O_{10}$ were determined by the second harmonic generation method, using cw Nd:YAG laser for both "type I" (ooe) and "type II" (eoe) phase matching configurations. The obtained values (d_{eff}^{I}=0.46±0.05 pm/V and d_{eff}^{II}=0.92±0.09 pm/V) are in good agreement with the results of relative measurements reported in the literature. The same value (0.92±0.09 pm/V) was found for d_{36} and d_{14} justifying experimentally the use of Kleinman's symmetry conjecture.

Dy, Er, Yb and Yb + Er doped $YAl_3(BO_3)_4$ (YAB) single crystals were grown by the top-seeded high temperature solution technique. Absorption and emission spectra of Dy^{3+} were determined in YAB:Dy crystals. The experimental oscillator strengths of the transitions were in good agreement with the Judd-Ofelt calculation performed. The dominant part of the emission corresponded to the $^4F_{9/2}$ – $^6H_{13/2}$ transition. Self-quenching of the luminescence and corresponding decrease of the decay time were observed at higher Dy-concentration due to activator-activator interactions. The narrow and polarization dependent emission lines, the relatively long lifetime (520 μs at RT) of the $^4F_{9/2}$ level, and the high quantum efficiency predict low threshold laser action in YAB:Dy.

The Stark components and their fine structure of the $^4I_{15/2}$ – $^4I_{13/2}$ and $^4I_{15/2}$ – $^4I_{11/2}$ infrared transitions of Er^{3+} were determined in YAB crystals by high resolution FTIR spectroscopy at 9 K. The observed very narrow absorption lines (down to half-width, FWHM = 0.14 cm^{-1}) indicated high crystal quality and uniform, single-site incorporation of the dopant. Some broadening and weak satellite lines occurred at high dopant concentration (12%). The absorption and emission spectra of Yb^{3+} were determined in YAB:Yb crystals. The emission spectra, excited with OPO laser, have shown an anti-Stokes transition at 10282 cm^{-1} in the 77 K measurements. The favorable overlap of the broad $^2F_{7/2}$ – $^2F_{7/2}$ Yb absorption band and the sharp $^4I_{15/2}$ – $^4I_{11/2}$ Er lines predicts the possibility of Yb-excitation – energy transfer – Er-emission mechanism.

Growth and study of stoichiometric $LiNbO_3$ single crystals. — The origin of light induced refraction index changes has been determined in Mg doped, congruent and stoichiometric $LiNbO_3$ by the combination of single-beam *Z*-scan method and CCD recording of the transmitted beam cross section. In the congruent $LiNbO_3$ samples (doped by Mg up to 5mol%) photorefraction dominates all among the non-linear effects. For the stoichiometric samples (doped with 2-5mol% Mg) the photorefraction is absent even at MW/cm^2 light intensity levels. The positive sign of the Z-scan traces, and the order of magnitude of the measured nonlinear refractive index (n_2^*) values of the Mg doped stoichiometric crystals indicate that the light induced change of the refractive index is of thermal origin and associated with nonlinear absorption.

The absolute values of the effective non-linear coefficients (d_{eff}) of $LiNbO_3$ crystals were determined for different [Li]/[Nb] ratio by using the second harmonic generation method. The experiments were carried out at room temperature with a cw Nd:YAG laser at "type I" (ooe) phase matching configuration both in xz and yz light propagation. The deduced values for the coefficients d_{31} and d_{22} were shown to be sensitive to the crystal composition and they increased by about 20 % when the [Li]/[Nb] ratio varied from 0.984 to 0.998.

Using high-resolution excitation and emission spectroscopy, the changes occurring in the optical transition of Er^{3+} ions in $LiNbO_3$ were investigated during the inversion of the ferroelectric axis. In stoichiometric crystals reconfiguration among different defect sites were found favoring those centers which have already been dominant in the as-grown sample. This reconfiguration was attributed to re-arrangement of the local charge compensators. We also found a small shift of the emission transition energy, which was consistent with an increase of the intrinsic electric field. The effect of domain inversion on the spectra of the Er^{3+} tracing element was also studied by site-selective spectroscopy. Significant modifications in the Er^{3+} emission spectra were revealed at specific excitation energies. These changes were used in a confocal luminescence microscope to image the ferroelectric domain structures. The method makes it possible the in situ observation of the domain inversion. The spatial and temporal resolution achieved (700 nm and 50 ms) is sufficient to study the dynamic behavior of the domain walls during domain inversion.

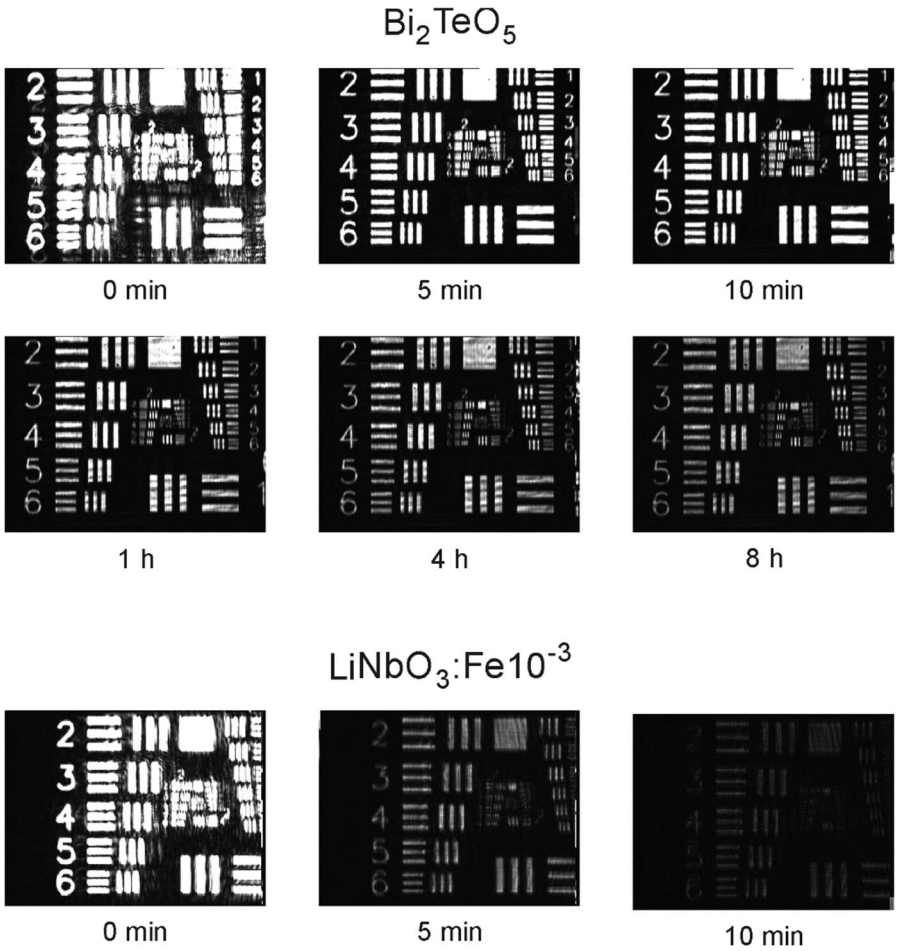
Growth and study of bismuth tellurite crystals. — Analog volume holograms of a two-dimensional test pattern were recorded in undoped Bi_2TeO_5 crystals by using a cw Nd:YAG laser at 532 nm. The holographic memory performance of Bi_2TeO_5 was compared to that of the generally used $LiNbO_3$:Fe crystals. In both crystals sharp contours, high contrast and resolution, and low background noise reflected the good quality of the analog holograms after recording. The photorefractive sensitivity of the undoped Bi_2TeO_5 was moderate, much below the performance of $LiNbO_3$:Fe.

The durability of the recorded holograms were tested in the dark (with 2s long sequential reading), and during permanent read-off by strong, 2mW, 532 nm laser beam. In Bi_2TeO_5, the recorded image showed a fast decaying initial section in the dark (up to about 10 min), after which the contrast has remained unchanged until the 50 h limit of the observation. This was in accordance with the former photorefractive observations of multi-step decay and self-fixing of the photorefractive signal. The dark decay of the image in $LiNbO_3$:Fe was of single exponential, without fixed fraction.

The self-fixed holograms in Bi_2TeO_5 were rather nonvolatile in the permanent read-out process. Using 2mW 532 nm laser exposure, the hologram remained readable after 8 hours. This means more than 10000 possible subsequent individual read-out (2s each). This is a unique performance, since under the same conditions, the hologram in the $LiNbO_3$:Fe crystals totally decayed within 15 min (Fig.1).

Page-oriented digital volume holograms were recorded in Bi_2TeO_5 and $LiNbO_3$:Fe crystals. The quality of the holograms was characterized by the bit-error-rate (BER), the fraction of mis-interpreted bits during reconstruction of the page. In our $LiNbO_3$:Fe crystals, the initial BER was close to 10^{-13}, better than the previous reports under same conditions, reflecting the utmost optical quality of the crystal. The starting BER in Bi_2TeO_5 was weaker, only 10^{-9}. During permanent read-out by 0.5 W/cm^2 reference beam, the initial BER in $LiNbO_3$:Fe decayed to the useless 10^{-2} value within 3 min. In Bi_2TeO_5, after an initial decay of about 10 min, the BER value remained 10^{-4} up to 45 min limit of the experiment. This demonstrated the self-fixing performance of Bi_2TeO_5, and the potential of application of the material in digital volume optical storage.

Gold and silver nano-clusters were produced in Bi_2TeO_5 by ion implantation using 800 KeV Au^+ and 450 KeV Ag^+ exposure at room temperature. The samples then were annealed at 600 ºC and 45O ºC, respectively. Strong, broad absorption bands appeared in the implanted crystals. The position and shape of the bands allowed us to calculate the dimension of the nanoparticles (2-10 nm). For Au+Ag double implantation, the formation of Au/Ag alloy type nano-clusters was observed.



Decay of volume holograms in Bi_2TeO_5 and $LiNbO_3$:Fe single crystals under permanent reading by 2mW, 532 nm laser beam.

Analytical spectroscopy. — Our analytical experience was employed in environmental experiments in cooperation with the University of Antwerp. Aerosol monitoring was performed in Flanders (6 different sites in and around Antwerp) by applying various sampling and size-fractionated separation of the suspended matter along the aerodynamic diameters, with a special care to $PM_{2.5}$ (fine respirable particulate matter). By using various analytical techniques, the map of Na^+, K^+, NH_4^+, Ca^{2+}, Mg^{2+}, F^-, Cl^-, NO_3^-, SO_4^{2-}, PO_4^{3-}, SO_3^{2-} and NO_2^- ion concentration distribution in the collected particles were prepared.

Determination methods were tested for the analysis of platinum group metals (PGMs) in various environmental compartments, originating from anthropogenic emission, mainly from the increasing application of catalytic converter units of modern vehicles. These experiments provided good basis for studying the influence of fine particles from indoor and outdoor aerosols on the chronic obstructive respiratory diseases in and around Antwerp. It was shown that the PGMs concentration has increased significantly in the last decades in diverse environmental matrices; like airborne particulate matter, soil, roadside dust and vegetation, river, coastal and oceanic environment. Generally, PGMs are referred to be inert and immobile. On the other hand, there is an evidence of spread and bioaccumulation of these species in the environment. Platinum content of road dusts, can be soluble. Consequently, it enters to the waters, soil, and finally, the food chain. The effect of chronic occupational exposure to Pt compounds is well documented, and certain Pt species are known to exhibit allergenic potential, but the toxicity of bio-available anthropogenic Pt is not clear.

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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, 1999-2003)

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).

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

4016/NATO/03. NATO Scientific Fellowship Program (L. Bencs, 2003). Partner: University of Antwerp,

HAS- Russian Academy Project 18. Investigation of crystal defects in broad forbidden band crystals (J. Janszky, contributor K. Polgár, 2002-4). Partner: Joffe Phys. Techn. Inst., St. Petrersburg

HAS- Russian Academy Project 19. Solid State lasers (A. Citrovszky, contributor K. Polgár, 2002-4). Partner: General Physics Institute, RAS, Moscow.

HAS-CNR joint project, Preparation and characterization of rare-earth doped crystals (L. Kovács, contributor: I. Földvári, 2001-3). Partner: Universita di Parma.

HAS-Polish Academy Pojekt 13. Investigation of structural defects in laser crystals. (A. Watterich, contributor: E. Beregi, 2002-4) Partner: Institute of Low Temperature and Structural Research, PAS, Wroclaw

ICAI-CT-2000-7029 KFKI-CMRC Centre of Excellence, WP12. Growth and complex study of optical crystals (J. Janszky, 2000-2003).

Long term visitors

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

— Armel Bahouka, Université du Metz, Metz, April 2003, 1 month (Host: K. Polgár)

Publications:

Articles

R.1. Domoniak-Dzik* G, Solarz* P, Ryba-Romanowsky* W, Beregi E, Hartmann E, Kovács L; Optical properties and laser potential of dysprosium doped $YAl_3(BO_3)_4$ crystal; *Rad Eff & Def Sol;* **157**, 1161-1165, 2002

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R.5. Klein* RS, Kugel* GE, Maillard* A, Polgár K, Péter Á; Absolute nonlinear optical coefficients of $LiNbO_3$ for near stoichiometric crystal compositions; *Opt Mater;* **22,** 171-174, 2003

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R.15. Kling* A, Soares* JC, Fichtner* PFP, Amaral* I, Zawislak* F, Földvári I, Péter Á; Creation of noble metal nanoclusters in bismuth tellurite; *Nucl Instr Meth Phys Res; B*. **206,** 653-656, 2003

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R.17. Bencs L, Ravindra* K, Van Grieken* R; Methods for the determination of platinum group elements originating from the abrasion of automotive catalytic converters *; Spectrochim Acta B;* **58,** 1723-1755, 2003

R.18. Bencs L, Szakács O, Szoboszlai* N, Ajtony* Zs, Bozsai* G; Characteristics of atomic absorption calibration curves with the transversely heated graphite furnace*; J Anal At Spectrom;* **18,** 105-110, 2003

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R.20. Polgár K, Péter Á, Ferriol* M; Phase relation in the growth of stoichiometric lithium niobate; *Phys Stat Sol(a);* accepted for publication

Conference proceedings

R.21. Földvári I, Péter Á, Polgár K, Berger* G, Denz* C; Growth and characterization of photorefractive oxide crystals. In: *9th International Conference on Photorefractive Effects, Materials and Devices, La Colle sur Loup, Nice, France, June, 2003*; OSA Trends in Optics and Photonics, Eds: P. Delaye, C. Denz, L. Mager, G. Montemezzani, Vol. **87,** pp.58-65, 2003

R.22. Berger* G, Müller* KO, Denz* C, Földvári I, Péter Á, Digital data storage in a phase-encoded holographic memory system: data quality and security. In: *Advanced Optical Storage, SPIE Photonics West '03 Conference, Jan Jose CA, January 2003*; SPIE Proc., Ed: H.J. Coufal. Vol. **4988,** pp. 104-111, 2003

See also S.1., S.2., S.6., S.9., S.10., S.11., S.13., S.14., S.18., S.24

S. CHARACTERIZATION AND POINT DEFECT STUDIES OF OPTICAL CRYSTALS

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

Microscopy of as-grown surface structure and composition of YAB crystals. — The surface microstructures observed by optical and scanning electron microscopy (SEM) on as-grown habit faces of undoped, Nd- and Cr-doped YAB single crystals showed both the {101} type pyramid and the {110} type prism faces to grow by layer-by-layer mechanism. The average surface density of dislocations causing small flat hillocks on the prism faces of crystals was found to be between 10^5 and 10^6 cm^{-2}. On the prism faces thin straight streaks, crystallographically well oriented, were also observed overlaping the growth hillocks, pointing to the presence of some inner planar defects, maybe microtwins.

The comparisons of the bulk crystal compositions measured by atomic absorption spectroscopy and near-surface compositions obtained by energy dispersive X-ray spectroscopy revealed concentration deficiencies of Y and Al matrix components related to the stoichiometric ones. These deficiencies were smaller in the near-surface regions developed during the final growth stages than in the bulk, as it was theoretically expected.

Point defects in oxide crystals. — Using electron paramagnetic resonance (EPR) and electron nuclear double resonance (ENDOR) new trapped electron and hole centres are characterised in $ZnWO_4$ single crystals produced by UV- or X-irradiation at 77 K. In undoped and Al-doped $ZnWO_4$ a W^{5+}-type defect is found which is stabilised by a nearby Al^{3+} impurity that is substituting for Zn^{2+}. In $ZnWO_4$:Al also three kinds of hole-type centres were studied: one of these is assigned to an O^- ion near a V_{Zn} - Al^{3+}_{Zn} complex, the second to an O^- ion near a V_{Zn}-OH^- pair. The third hole-type defect shows quartet SHF splitting (I=3/2) with a 100 % abundant nucleus and therefore the O^- in this centre is most likely stabilised by a Na^+ impurity. Complete sets of EPR parameters are compared for trapped electron and trapped hole centres including previously characterised defects.

The photostimulated luminescence (PSL) of Mo, Fe doped and undoped $ZnWO_4$ crystal was studied. The observed PSL is caused by the recombination of optically released self-trapped holes (in undoped crystals) or the holes perturbed by impurity ions (in doped crystals) with electronic centres of unknown nature. The creation spectrum of self-trapped holes, i.e. the PSL excitation spectrum, was measured in the energy region of 4-30 eV. The defined energy region of one electron-hole pair creation (E=6-12 eV) and that of multiple electron-hole pair creation (E>12 eV) are shown to be consistent with the known value of the energy gap (E_g=5.7 eV) of $ZnWO_4$.

Cu and Eu doped $Li_2B_4O_7$ has been characterised by steady-state and time-resolved photoluminescence, radioluminescence and optical absorption spectroscopy. The effect of dopant concentration and host modification was described.

Optical absorption and simultaneous EPR measurements have been applied to characterise Ti^{3+} centres in thermochemically reduced Ti and/or Mg doped $LiNbO_3$ single crystals. The Ti^{3+} absorption bands have been identified and their redshift upon Mg codoping has been ascribed to the change of the incorporation of Ti from the Li to the Nb site. Charge transfer

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processes essential for holographic writing and readout involving polaronic states and also Ti^{3+} centres have been characterized.

Hydroxyl ion (OH^-/OD^-) absorption has been observed in as-grown and thermally treated $LaGaO_3$ crystals at 9K at 3521 cm^{-1} / 2601 cm^{-1} wavenumbers. The anharmonicity parameters of the stretching vibration and the possible lattice site of the OH^- ions have been determined. A structural phase transition of $LaGaO_3$ has also been detected at 418 K using the Fourier transform infrared (FTIR) absorption technique.

The presence of water molecules has been shown in $CsLiB_6O_{10}$ crystals by FTIR spectroscopy. The absorption bands related to the normal modes of the water molecule and their combinations and overtones have been assigned. The water molecule occupies the large Cs channel in the crystal lattice as concluded from the polarization absorption measurements. The in- and out-diffusion of water has been studied as a function of the humidity and temperature of the surrounding atmosphere. The dc conductivity of the crystals in the 50 – 750 ºC range followed the Arrhenius law and showed only weak anisotropy.

Investigation of X-ray storage phosphors. — Photoluminescence studies in Ce^{3+} activated $BaBr_2$ single crystal storage phosphors have shown the presence of three types of Ce^{3+} centres differing in charge compensation as suggested also by EPR. Two types of charge-compensated centres are also active as recombination sites in the photostimulated luminescence process used for the readout of stored X-ray images both in these crystals and in fluorobromozirconate glass ceramics containing nanocrystalline $BaBr_2$ phases.

Thermal fixing and spatial distribution of wave mixing hologram in $LiNbO_3$. — The angular dependence of the scattering intensity was measured to determine the optimal conditions for the application of the holographic scattering method. We found a simple empirical form that fits well both the measurements and the theoretical function and very suitable for mathematical calculations. It was shown by using this empirical form that the integral loss of transmitted intensity is practically insensitive to the dependence of the relaxation time on the grating spacing for samples with high free ion concentration (e.g. as-grown crystals).

Using our four-wave mixing topographic set-up, we measured the build-up and the translation of two-wave mixing soliton-like diffraction efficiency distributions. We found that the build-up of the peek - after a fast and very week transient penetration at the edge of the sample - develops at the stationary location and has the same shape with increasing magnitude.

Design, recording and microscopic observation of optical gratings. — Transmission and reflection phase gratings were designed and recorded in glass substrates via ion implantation. Phase contrast and interference microscopy were used for direct observation of phase holograms recorded holographically in silver halide emulsions, photopolymers and photorefractive crystals. Refractive index modulation in silver halide phase holograms as a function of bias exposure and fringe visibility and grating spatial frequency was determined. Lin-curves (nonlinear characteristics) of the same holograms were derived form the results of the refractive index measurements using coupled wave theory.

History of Science. — The bequest of Prof. Zoltan Gyulai (1887-1968) in the Archive of the Hungarian Academy of Sciences was searched for finding the original manuscripts of his famous papers in the field of solid state physics. Many personal data could be collected. The event chronology of the Gyulai-Tarján crystal physics school was supplemented with private notes recently found.

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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 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).

TéT German-Hungarian Intergovernmental S&T Cooperation, (D-11/2001) Composition-dependent properties of oxide crystals for holographic applications (G. Corradi, 2002-2003)

TéT Austrian-Hungarian Intergovernmental S & T Cooperation (A-8/2001): Minerals and synthetic crystals for optical applications (L. Kovács, 2002-2003)

TéT Ukrainian-Hungarian Intergovernmental S & T Cooperation (UK-3/2002): Investigation of point defects and OH groups in $LiNbO_3$ and $CdWO_4$ crystals (L. Kovács, 2003-2004)

TéT British-Hungarian Intergovernmental S & T Cooperation (GB-11/2003): Modelling of crystal defects in photorefractive materials (L. Kovács, 2003-2005)

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

HAS – Polish Academy of Sciences joint project: Investigation of structural defects in laser crystals (L. Kovács, 2002-2004)

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)

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

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Articles

S.1. Kappers* LA, Gilliam* OR, Bartram* RH, Watterich A, Földvári I; Discovery of a self-trapped-electron center in α-TeO_2; *Radiation Effects and Defects in Solids*; **157**, 671-676, 2002

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S.13. Watterich A, Hofstaetter* A, Scharmann* A, Szakács O; Al- and OH-related paramagnetic impurity centres in UV – or X-irradiated $ZnWO_4$ single crystals; *J Phys: Condensed Matter*; **15**, 7073 –7084, 2003

S.14. Bugaychuk* S, Kovács L, Mandula G, Polgár K, Rupp* RA; Nonuniform dynamic gratings in photorefractive media with nonlocal response; *Physical Review*; **E67**, 046603/1-8, 2003

S.15. Bányász I; Spatial frequency dependence of the nonlinear characteristics of bleached silver-halide holographic materials; *Optics Communications*; **225**, 269-275, 2003

S.16. Bányász I; Direct measurement of the refractive index profile of phase gratings, recorded in silver halide holographic materials by phase-contrast microscopy; *Applied Physics Letters*; **83,** 4282- 4284, 2003

S.17. Corradi G, Secu* M, Schweizer* S, Spaeth* J-M; Luminescence properties of the X-ray storage phosphor $BaBr_2:Ce^{3+}$; *J Phys: Condensed Matter*; accepted for publication

S.18. Corradi G, Meyer* M, Kovács L, Polgár K; Gap levels of Ti^{3+} on Nb or Li sites in $LiNbO_3$:(Mg):Ti single crystals and their effect on charge transfer processes; *Applied Physics B*; accepted for publication

Articles in Hungarian

S.19. Hartmann E, Janszky J, Rontó* Gy; Turchányi György (1913-2001); (G. Turchanyi, in Hungarian); *Fizikai Szemle;* **53**, 109-110, 2003

Conference proceedings

S.20. Bugaychuk* S, Rupp* RA, Mandula G, Kovács L; Soliton profile of the dynamic grating amplitude and its alteration by photorefractive wave mixing; In: *Photorefractive Effects, Materials, and Devices, La Colle sur Loup, France, 17-21 June 2003; OSA TOPS*; **87**, 404-409, 2003

S.21. Bányász I, Fried* M, Dücső* C, Vértesy* Z; Phase grating fabrication in glass via ion implantation; In: *Symposium Photonics Fabrication Europe 2002, Brugge, Belgium*; Ed.: Giancarlo C. Righini; *Proc. SPIE*; **4944,** pp. 171-182, 2003

S.22. Bányász I; Measurement of nonlinear characteristics of silver halide holographic materials by phase-contrast microscopy; In: *Symposium Electronic Imaging 2002, Santa Clara, CA, USA*; Eds.: Tung H. Jeong, Sylvia H. Stevenson; *Proc. SPIE*; **5005,** pp.86-94, 2003

S.23. Bányász I; Measurement and modelling of the full nonlinear characteristics of silver-halide holographic recording materials; In: *Symposium Electronic Imaging 2002, Santa Clara, CA, USA*; Eds.: Tung H. Jeong, Sylvia H. Stevenson; *Proc. SPIE*; **5005,** pp. 55-64, 2003

Conference proceedings in Hungarian

S.24. Malicskó L, Tóth A*, Beregi E, Horváth V; Mikroszkópos eset tanulmányok egyes YAB egykristályokon; (Microscopic case-studies on some YAB single crystals); In: *"Kvantumelektronika 2003", Proc. of the 5th National Symposium on Quantum Electronics, 21. October 2003, Budapest, Hungary*; Ed: Varró S, (ISBN 963 372 629 8), p.14, 2003

See also R.1., R.9., R.19.

T. NONLINEAR AND QUANTUM OPTICS

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

Quantum interference. — We have proposed an efficient nonlinear frequency conversion scheme, which performs the conversion from the injected to the generated pulses in a phaseonium medium with unit efficiency. We have worked out the coherent control of the quantum state of degenerate, two-level, angular-momentum-state systems in the M and W coupling configurations. In particular, we have shown how the ellipticity and the shape of the exciting pulse should be chosen to achieve prescribed final population distributions. We have worked out a robust control scheme to manipulate the quantum state of a SQUID qubit.

Quantum optics of microstructures, cavity quantum electrodynamics. — We have designed an optical microcavity which can be integrated on an atom chip surface and permits unambiguous detection of a single atom with 10 microsecond integration time without causing the atom to undergo spontaneous emission. We found a giant Lamb shift, accompanied by greatly enhanced light scattering, of atoms embedded in microscopic optical waveguides driven slightly below the cutoff frequency of a new transverse branch of propagating modes.

We found that a high-finesse resonator with its axis transverse to the standard Doppler cooling scheme extends the trapping times to the unexpectedly long range of seconds. We showed that the trapping time as well as the trapping position exhibits an interference effect, as being sensitive to the relative phase of the cooling laser beam and the weak cavity pump field.

Quantum information, entanglement and teleportation. — The antilinear operator representation of bipartite pure entangled states (of the relative state formulation of quantum mechanics) allows us to easily interpret various protocols of quantum information theory including teleportation or entanglement swapping utilizing nonmaximally entangled resources: effects of Bell like measurement processes on shared entangled states can be simply obtained by 'concatenating' the corresponding antilinear operators. To optimize imperfect schemes we introduced the notion of 'entanglement matching,' a condition for the resources envolved in the scheme.

We have studied the possibility of simulating an amplitude damping channel on a programmable quantum gate array (quantum processor). We have found that the process is always accompanied by an additional phase damping which has been explained in terms of information flow in the process.

Nuclear motion in molecules: dynamics and spectroscopy. — The rotational-internal rotational motion and the related spectra of molecules possessing some special geometrical symmetry is usually described and analyzed with the help of the rho-axis-system hamiltonian. We have extended this hamiltonian to molecules with no restriction on symmetry and type of large amplitude internal motion.

High-quality ab initio quantum chemical methods, including higher-order coupled cluster and full configuration interaction benchmarks, have been employed to obtain the best technically possible value for the standard enthalpy of formation of CH_2.

[#] Ph.D student

Although one cannot directly relate any Gaussian quadrature to general basis functions, the discrete variable representation derivable with such basis sets via the transformation method is, as we have proved, of Gaussian quadrature accuracy.

We have calculated ab intio a benchmark-quality torsional potential fully reflecting the symmetry and internal rotation dynamics of acetaldehyde in the energy range probed by spectroscopic experiments in the IR and MW regions.

Quantum field theory in singular media. — Quantum field theory and general relativity are two fundamental theories of modern physics. Experimental studies of quantum field theory in curved space-time, however, are not yet possible and seem extremely difficult. For example, the famous prediction of Hawking, the emergence of thermal radiation from the event horizon of a black hole, could not have been observed up till now.

An alternative way of studying Hawking radiation and related phenomena is based on the analogy between gravity and moving media. Two decades ago Unruh pointed out the existence of an effective metric for sound waves in moving fluids. Recent advances in controlling quantized wave propagation in various media in the laboratory have revived interest in analogue Hawking radiation. Propagation of quantized sound-like excitations in moving Bose-Einstein condensates is a promising candidate for such experiments. The event horizon corresponds to the surface where the fluid velocity crosses the local speed of sound. That point corresponds to singular behavior in the wave equation. The wave catastrophe is avoided by the breakdown of the sound wave approximation and thus the effective metric. The related phenomenon in general relativity is known as the notorious trans-Planckian problem.

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Viktor Szalay	viktor@szfki.hu
András Vukics	vukics@optics.szfki.kfki.hu

Grants and international cooperations

OTKA T043079	Moving atoms and molecules in strongly-coupled radiation fields (P. Domokos, 2003-2006)
OTKA T043287	Adiabatic control in quantum optics and quantum informatics (Z. Kis, 2003-2006)
OTKA T034484	Application of nonclassical light in fundamental physical problems and in optical measurement methods (J. Janszky, 2001-2003)
OTKA T034327	Reconstruction of vibrational 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 rotational-torsion spectrum of molecules with asymmetric top and asymmetric frame, and analysis of overlapping spectral bands by filter diagonalization (V. Szalai, 2001-2003)

Long term visitor

— Emmanuel Paspalakis, University of Patras, Greece, July, October (host: J. Janszky)

Publications

Articles

T.1. Domokos P, Ritsch* H; Collective cooling and self-organization of atoms in a cavity; *Phys Rev Lett*; **89**, 253003/1-4, 2002

T.2. Ádám P, Kárpáti A, Gawlik* W, Janszky J; Competitive stochastic noises in coherently driven two-level atoms and quantum interference; *J Opt B: Quantum Semicl Opt*; **5**, S221-S227, 2003

T.3. Császár* AG, Leininger* ML, Szalay V; The standard enthalpy of formation of CH_2; *J Chem Phys*; **118**, 10631-10642, 2003

T.4. Domokos P, Ritsch* H; Mechanical light effects in optical resonators; *J Opt Soc Am B*; **20**, 1089–1122, 2003

T.5. Horak* P, Klappauf* BG, Haase* A, Folman* R, Schmiedmayer* J, Domokos P, Hinds* EA; Possibility of single-atom detection on a chip; *Phys Rev*; **A67**, 043806/1-9, 2003

T.6. Horak* P, Domokos P, Ritsch* H; Giant lightshift of atoms near lossy multimode optical micro-waveguides; *Europhys Lett*; **61**, 459-465, 2003

T.7. Janszky J, Asbóth J, Gábris A, Vukics A, Koniorcyzk M, Kobayashi* T; Two-mode Schrödinger cats, entanglement and teleportation; *Fortschr Phys*; **51**, 157-171, 2003

T.8. Kárpáti A, Kis Z; Adiabatic creation of coherent superposition states via multiple intermediate states; *J Phys B*; **36**, 905-919, 2003

T.9. Kárpáti A, Ádám P, Gawlik* W, Lobodzinski* B, Janszky J; Quantum trajectory approach to stochastically-induced quantum interference; *Fortschr Phys*; **51**, 179-185, 2003

T.10. Kis Z, Paspalakis* E; Enhancing nonlinear frequency conversion using spatially dependent coherence; *Phys Rev*; **A68**, 043817/1-9, 2003

T.11. Koniorczyk M, Buzek* V; Simulation of exponential decay on simple quantum circuits: a case study; *J Opt B: Quantum Semicl Opt*; **5**, S329-S332, 2003

T.12. Kurucz Z, Koniorczyk M, Ádám P, Janszky J; An operator description of entanglement matching in quantum teleportation; *J Opt B: Quantum Semiclass Opt*; **5**, S627-S632, 2003

T.13. Leonhardt* U, Kiss T, Ohberg* P; Bogoliubov theory of the Hawking effect in Bose-Einstein condensates; *J Opt B: Quantum Semiclass Opt*; **5**, S42-S49, 2003

T.14. Leonhardt* U, Kiss T, Ohberg* P; Theory of elementary excitations in unstable Bose-Einstein condensates; *Phys Rev*; **A67**, 033602/1-11, 2003

T.15. Szalay V, Császár* AG, Santos* J, Ortigoso* J: Rho-axis-system Hamiltonian for molecules with one large amplitude internal motion; *J Chem Phys*; **118**, 6801-6805, 2003

T.16. Szalay V, Czakó* G, Nagy* A, Furtenbacher* T, Császár* AG: On one-dimensional discrete variable representations with general basis functions; *J Chem Phys*; **119**, 10512-10518, 2003

T.17. Vukics A, Asbóth J, Meszéna* G; Speciation in multidimensional evolutionary space; *Phys Rev*; **E68**, 041903/1-10, 2003

T.18. Császár* AG, Szalay V, Senent* ML; Ab initio torsional potential and transition frequencies of acetaldehyde; *J Chem Phys*; accepted for publication.

T.19. Gawlik* W, Lobodzinski* B, Ádám P, Kárpáti A, Janszky J; Stochastically-induced quantum interference in coherently driven two-level system; *Quantum Electronics (Acta Phys Hung B)*; accepted for publication.

T.20. Kárpáti A, Ádám P, Janszky J; A method for calculating two-time correlation functions in the quantum trajectory approach; *J Opt B: Quantum Semiclass Opt*; accepted for publication.

T.21. Kis Z and Paspalakis* E; Arbitrary rotation and entanglement of flux SQUID qubits; *Phys Rev*; accepted for publication.

T.22. Kiss T, Ádám P, J. Janszky J; Gauss filtered back projection for the reconstruction of the Wigner function; *Quantum Electronics (Acta Phys Hung B)*; accepted for publication.

T.23. Paspalakis* E and Kis Z: Novel Nonlinear Optical Response of Phase Coherent Media, *Rec Res Dev Opt*; accepted for publication.

T.24. Vitanov* NV, Kis Z, and Shore* BW; Coherent excitation of a degenerate two-level system by an elliptically polarized laser pulse; *Phys Rev*; accepted for publication.

T.25. Vukics A, Domokos P, Ritsch* H; Multidimensional and interference effects in atom trapping by a cavity field; *J Opt B: Quantum Semiclass Opt*; accepted for publication.

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 28th of February 2004. In the current reporting period the implementation of the project goals has continued successfully. As a result 92 scientific papers have been published, among them 89 papers in international journals (e.g. in the Physical Review B and E as well as in the Physical Review Letters), 3 papers have been published in conference proceedings.

So far since the beginning of the project we have employed 86 foreign scientists from 10 different countries as long term visitors for 212 months altogether, 90 foreign scientists visited our centre for a short period of time. We have organised 19 international conferences, workshops and have purchased durable equipment for 23179 Euro. Several research teams take part in framing proposals for the 6th Framework Programme, also there are two projects that have now passed the first phase of evaluation.

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 scientist are continuously studying these changes in order to ensure successful participation.

EDUCATION

Graduate and postgraduate courses, 2003

— Electrodynamics of continuous media (F. Woynarovich, ELTE[3])

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

— Advanced solid state physics III. (J. Sólyom, ELTE)

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

— Phase transformations and critical phenomena (F. Iglói, SZTE)

— Statistical physics (P. Fazekas, BUTE[5])

— Magnetism II. (P. Fazekas, BUTE)

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

— Optical properties of solid state (I. Tüttő, ELTE)

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

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

— Amorphous and crystalline materials (regular lecture for 4th grade Engineering Physics Students, P. Deák*, S. Kugler* and T. Kemény, BUTE)

— Modern theory of nucleation (L. Gránásy, ELTE)

— Macromolecules (S. Pekker, ELTE)

— Spectroscopy and materials structure (K. Kamarás, BUTE)

— Methods in materials science (K.Kamarás, BUTE)

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

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

— Superconductivity (G. Kriza, BUTE)

— Physics of liquid crystals and polymers (Á. Buka and N. Éber, ELTE)

— Pattern formation in complex systems (Á. Buka, ELTE)

— Liquid crystals, their chemistry and chemical physics (K. Fodor-Csorba, ELTE)

— Nanophase metals (I. Bakonyi, ELTE)

— Advanced material technology (G. Konczos, BUTE)

— Introduction to materials science (G. Konczos, BUTE)

— NMR spectroscopy (K. Tompa, BUTE)

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

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

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[3] ELTE = Loránd Eötvös University, Budapest

[4] SZTE = University of Szeged

[5] BUTE = Budapest University of Technology and Economics

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

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

— Growth, processing and characterization of nonlinear optical crystals (in: Applied Lasertechnics, I. Földvári, BUTE)

— Theories of Crystal Growth (L. Malicskó, BUTE)

— Microscopy in Materials Science (L. Malicskó, BUTE)

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

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

— Quantum Mechanics I. (P. Ádám, PTE[6])

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

— Thermodynamics and statistical physics (P. Ádám, PTE)

— Atom and ion traps (P. Ádám, PTE)

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

— Mechanics (J. Janszky, PTE)

— Quantum optics (J. Janszky, PTE)

— Introduction to computer-aided measurement data processing I. (Basics) (M. Koniorczyk, PTE)

— Introduction to computer-aided measurement data processing II. (Digital Signal Processing) (M. Koniorczyk, PTE)

— Vector calculus 3 (Z. Kurucz, PTE)

— Vector calculus 4 (Z. Kurucz, PTE)

— Informatics I. (Z. Kurucz, PTE)

Laboratory practice and seminars

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

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

— Physics laboratory I-II. (L. Gránásy, BUTE)

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

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

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

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

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

— Computing in chemistry (L. Pusztai, ELTE)

[6] PTE = University of Pécs

— Laboratory practices in physics IV. (L. Temleitner, BUTE)

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

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

— Introduction to physics (K. Lengyel, PTE)

— Vector calculus II seminar (K. Lengyel, PTE)

— Vector calculus IV seminar (K. Lengyel, PTE)

— Theoretical physics seminar (P. Ádám, PTE)

— Mechanics II seminar (A. Gábris, PTE)

— Calculus and linear algebra seminar I-II. (M. Koniorczyk, PTE)

— Quantum Mechanics seminar (M. Koniorczyk, PTE)

Diploma works

— L. Temleitner (BUTE): Neutron diffraction and computer simulation studies of the structure of molecular liquids (Consultant: L. Pusztai)

— M. Fábián (Babes-Bolyai University, Cluj): Structural characterization of borosilicate glasses (Consultant: E. Sváb)

— R. Sinka (Babes-Bolyai University, Cluj): The effect of CeO_2 on the structure of borosilicate glasses in dependence of ZrO_2 content (Consultant: E. Sváb)

— B. Rózsa (ELTE): Development and use a two photon microscope for measurement of neural networks (Consultant: R. Szipőcs)

— J. Asbóth (ELTE): Correlated motion of atoms in an optical resonator (Consultant: P. Domokos)

— A. Vukics (ELTE): Three-dimensional, dissipative motion of atoms in optical resonators (Consultant: P. Domokos)

Ph. D. students

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

Z. Jurek (BUTE): 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 (BUTE): Instabilities and convective patterns in liquid crystals. (Supervisor: Á. Buka)

E. Kochowska (Poland): Electrohydrodynamics in nematics (Supervisor: Á. Buka).

A. Bárdos (BUTE): 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 (BUTE): NMR study of low-dimensional metals (Supervisor: G. Kriza)

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

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

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

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

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

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

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

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

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

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

N.K. Székely (ELTE): SANS investigation of molecular liquids (Supervisor: L. Rosta)

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

L. Temleitner (BUTE): Diffraction and computer simulation studies of disordered molecular systems (Supervisor: L. Pusztai)

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

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

P. Hartmann (ELTE): Heavy-particle processes in low-pressure gas discharges (Supervisor: Z. Donkó)

P. Gál (BUTE): Development of light scattering instruments (Supervisor: A. Czitrovszky)

M. Füle (SZTE): Optical Absorption Investigation of Hydrogenated Amorphous Carbon Films (Supervisor: M. Koós)

D. Oszetzky (BUTE): Application of quantum-optical measurement methods (Supervisor: A. Czitrovszky)

S. Tóth (SZTE): Optical Absorption Investigation of Hydrogenated Amorphous Carbon Films (Supervisor: M. Koós)

L. Vámos (BUTE): Statistics of scattered light (Supervisor: P. Jani)

M. Veres (BUTE): Physical Properties of Graphitic Carbon Nano-Structures (Supervisor: I. Pócsik)

A. Bányász (ELTE): Femtochemistry (Supervisor: R. Szipőcs)

A. Lukács (PTE): Fluorescence spectroscopy for biomedical studies (Supervisor: R. Szipőcs)

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

T. Ujvári (BUTE): High capacity and fidelity holographic recorders specified by multiplexing and security measures (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)

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

A. Vukics (SZTE): Dissipative motion of atoms in strongly-coupled light fields (Supervisor: P. Domokos)

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

Dissertations

K. Pencz: Dynamics of correlated electron systems (D.Sc., Hungarian Academy of Sciences)

G. Bánó: Metal ion lasers in hollow cathode discharges (Ph.D., SZTE)

K. Kutasi: Hybrid modeling of basic phenomena in cold cathode glow discharges (Ph.D., SZTE)

M. Koós: Luminescence, Metastability and Localization in Amorphous Carbon and Amorphous Silicon Thin Films (D.Sc., Hungarian Academy of Sciences)

P. Jani: Study of the dynamics of nanometer-scale particles and displacements by quantum limited detection (D.Sc., Hungarian Academy of Sciences)

A. Nagy: Development of Aerosol Particle Counters and their application (Ph.D., BUTE)

S. Lakó: Investigations in femtosecond nonlinear optics (Ph. D., JATE)

M. Koniorczyk (SZTE-PTE): Quantum teleportation on generic Hilbert spaces and in Optics, (Supervisor: J. Janszky)

AWARDS

— F. Woynarovich, Széchenyi Professorship (2000-2003)
— A. Sütő, Physics Award of the H.A.S. (2003)
— Ö. Legeza, Bolyai Grant (2000-2003)
— J. Kollár, Széchenyi Professorship (2000-2003)
— L. Gránásy, Széchenyi Professorship (1999-2003)
— M. Bokor, Bolyai Grant (2001-2004)
— L. Péter, Young Researcher Award of the Hungarian Academy of Sciences (2003)
— L. Péter, SZFKI Annual Award for Applied Research (2003)
— I. Bakonyi, SZFKI Annual Publication Award (2003)
— G. Konczos, Diploma of Merit of the Secretary General, H.A.S. (2003)
— L. Pusztai, Széchenyi Professorship (2000-2003)
— Z. Donkó, SZFKI Annual Pubilaction Award (2003)
— G. Bánó, SZFKI Annual Award for Applied Research (2003)
— R. Szipőcs, ICO/ICTP[7] Award (2003)
— I. Földvári, Széchenyi Professorship, (2000-2003)
— J. Janszky, Simonyi Károly Award (2003)
— P. Domokos, Bolyai Grant (2003-2006)
— T. Kiss, Bolyai Grant (2003-2004)
— Z. Kis, Bolyai Grant (2001-2003), (2003-2004)
— J. Asbóth, OTDK National Conference of Student Research, 3. prize (2003)
— A. Vukics, OTDK National Conference of Student Research, 1. prize (2003)
— A. Vukics, Pro Scientia Gold Medal (2003)

[7] ICO-ICTP: International Commission for Optics, International Centre for Physics

CONFERENCES

— **2nd Central European Neutron Training Course, 07-11 April 2003, Budapest.** The course provided both valuable scientific and practical information on neutron scattering techniques and introduced the participants – future users, most of them coming from Central European countries (31 participants from 10 countries) – to the possibilities offered by the facilities of Budapest Neutron Centre, one of the most important large scale facilities in the region.

— The 2nd RMC Conference with the title '**The First Fifteen Years of Reverse Monte Carlo Modelling**' was held in Budapest, 9-11 Ocober, 2003 (Organiser: L. Pusztai). All aspects of diffraction- and EXAFS-based structural modelling were discussed by leading experts of the field, arriving from 11 countries. In addition to the 25 lectures, a poster session was also organised. The meeting was preceeded by a one day 'Reverse Monte Carlo tutorial' which was attended by about 20 people. A collection of review and original articles will serve as proceedings of the meeting, to be published in Journal of Physics: Condensed Matter.

— The "**Nuclear Methods in Studying Thin Films and Heterostructures**" workshop was held at 14th-15th November, with 55 participants. Internationally renowned experts from the EU and Candidate Countries has given state of art reports about the recent developments of research in the field of multilayers and granular materials. Besides the classical nuclear methods (ion beam analysis, neutron scattering, Mössbauer spectroscopy and muon spectroscopy) many other techniques were also discussed. Special mention must be made of electron microscopy which is capable of atomic level characterization of nanostructures and magnetotransport studies, which contribute to the understanding of the magnetic properties of nanosystems - a topic of most intensive research motivated both by academic and applied interest

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