ANNUAL REPORT

2004

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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of the Hungarian Academy of Sciences

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ANNUAL REPORT 2004

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

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Dear Reader,

It is my pleasure to hand over the 11th edition of the Annual Report of the Research Institute for Solid State Physics and Optics in 2004.

Our institute was founded by the Hungarian Academy of Sciences in 1981 as part of the Central Research Institute for Physics. In 1992 it 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 the 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 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.

The institute employs 183 people, among them approximately 110 scientists. During recent years more and more young researchers have joined our institute, so the employees' age distribution changed favourably. This and other statistics are given in the Key figures.

During the last year some of our co-workers were honoured with different awards and nominations. Imre Vincze, a senior scientist was elected as Corresponding Member of the Hungarian Academy of Sciences. One of our young co-workers Péter Domokos has been awarded the Talentum Prize by the Hungarian Academy of Sciences and a private foundation. Traditionally the Institute issues awards for publication and applied research activities. In 2004 the publication prize was won by László F. Kiss and Tamás Pusztai, while the applied research prize was shared by Pál Mezei and Tamás Cserfalvi.

We sorrowfully regret the loss of several outstanding co-workers this year. Rudolf Voszka — former leader of the Crystal Physics Laboratory — passed away after a long illness. Three of our senior scientists Mihály Jánossy, István Pócsik and Zsolt Szentirmai died in their creative ages. We keep in mind their essential contributions to the progress of laser physics and materials science.

This year 199 papers were published in high quality international journals and 44 papers in conference proceedings or books. The number of these publications is more than that of the previous years.

The research activity is financed by the Hungarian Academy of Sciences and by national and international research funds like the Hungarian National Research Fund (OTKA), the National Research and Development Program (NKFP), and also through individual projects.

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 Commission. The program has been running for four years. A description of the work conducted at the Centre can also 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 an important role in our research activity. Now the share of these international resources in our budget is about 5 % (see Key figures).

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

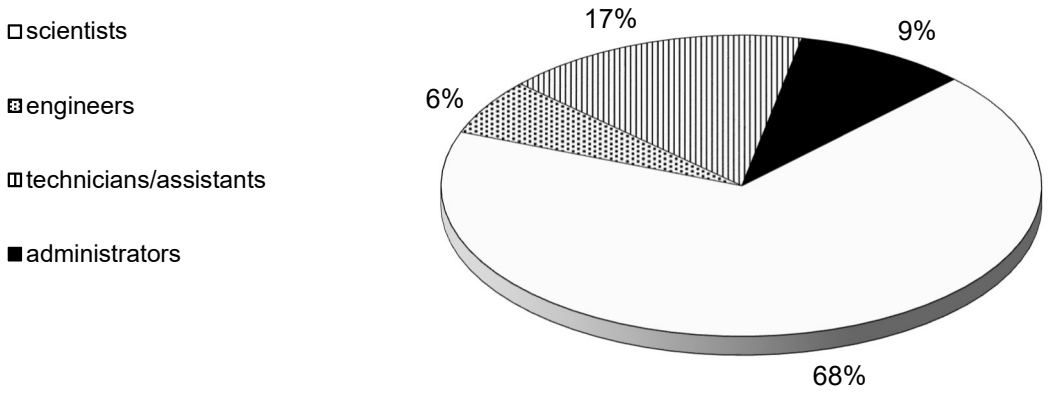
János Kollár

Director

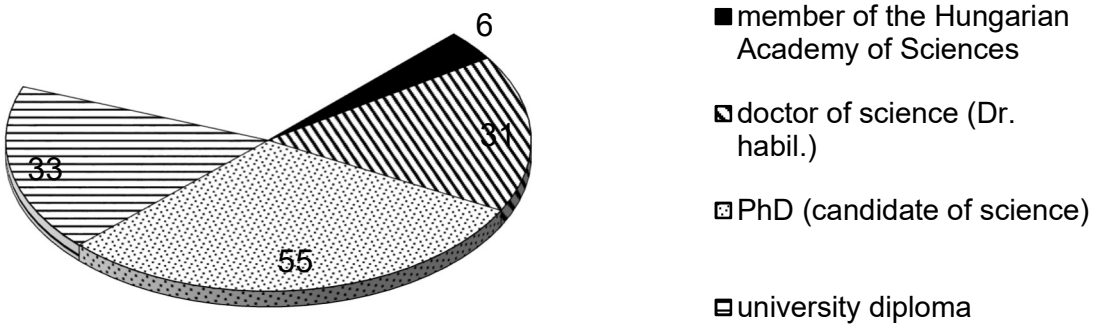
Key figures

Permanent staff of the Institute: 183 employees. Its distribution:

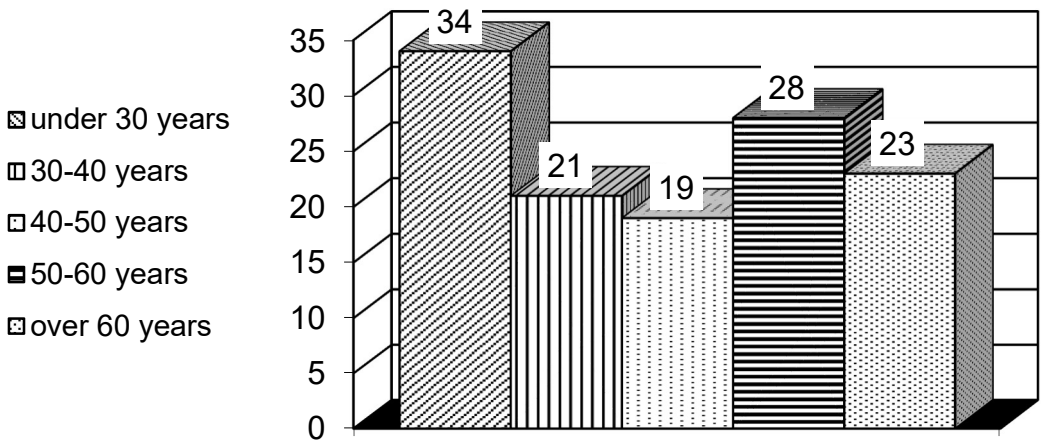
a) by professions:



b) by scientific titles/degrees:

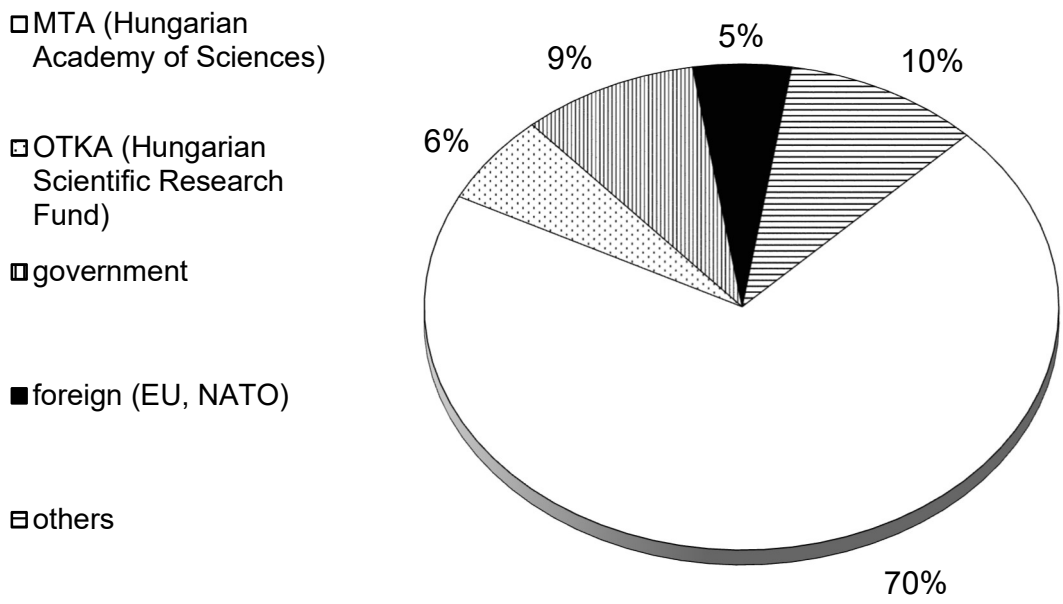


c) by ages:

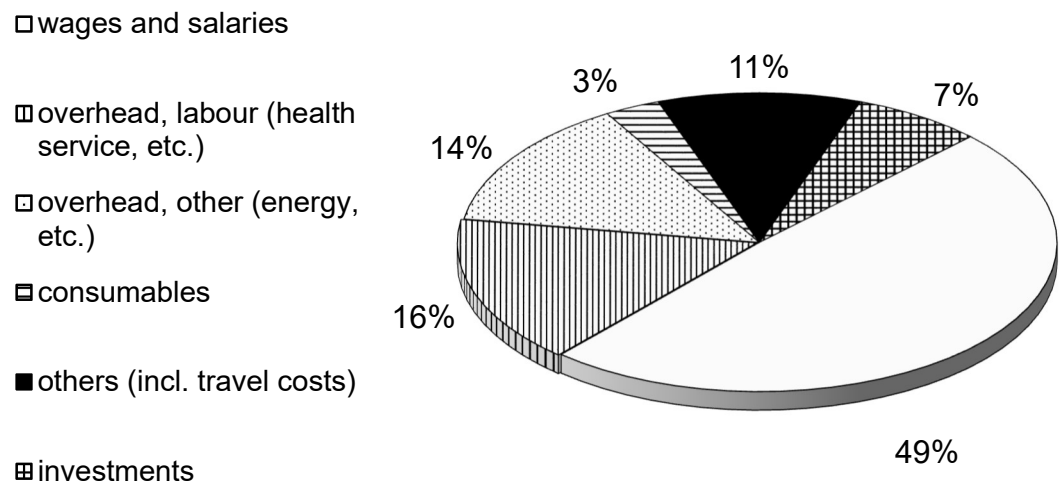


Financial management

a) Sources of operation costs:



b) Distribution of expenditures:



Structure of the Research Institute for Solid State Physics and Optics

A. STRONGLY CORRELATED SYSTEMS

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

Low dimensional fermionic and magnetic models. — We continued the application of quantum-information-theory concepts to improve the density-matrix renormalization group (DMRG) method. We have studied the quantum data compression for finite quantum systems where the site density matrices are not independent, i.e., the density matrix cannot be given as direct product of site density matrices and the von Neumann entropy is not equal to the sum of site entropies. Using the DMRG method for the 1-d Hubbard model, we have shown that a simple relationship exists between the entropy of the left or right block and dimension of the Hilbert space of that block as well as of the superblock for any fixed accuracy. The information loss during the DMRG procedure has been investigated and a more rigorous control of the relative error has been proposed based on Kholevo's theory. A sum rule which relates site entropies and the total information generated by the renormalization procedure has also been given which serves as an alternative test of convergence of the DMRG method.

We have further developed the dynamically extended active space (DEAS) procedure for the quantum chemistry version of DMRG (QC-DMRG). This new initialization procedure yields very accurate results even after the first-half sweeps of the DMRG method and reduces the computational time by an order of magnitude allowing us to carry out the largest QC-DMRG calculations up to date. The effect of site ordering has been further investigated and a more efficient ordering procedure has been proposed based on the competition of interaction localization and entanglement localization.

We have studied the possibility of the Mott metal-insulator transition in the SU(N) generalization of the one-dimensional Hubbard model. We have shown, using analytical perturbative renormalization group calculation that in the half-filled case the system is gapped for arbitrary on-site Coulomb repulsive, just as in the usual SU(2) model, even though the separation of charge and spin degrees of freedom, which makes the physics simple in the SU(2) case, does not hold for $N > 2$.

We have completed the study of the O(1) contributions of the saddle point fluctuations to the free energy of Bethe Ansatz systems. We developed a functional-integral method to calculate this contribution, and we have found, that it is determined by the energy of the particles and the scattering phase-shifts. The structure of these corrections is different whether periodic boundary condition is chosen or a finite system with open boundaries is studied.

Low dimensional and frustrated magnetic systems. — Magnetization plateaux, visible as anomalies in magnetic susceptibility at low temperatures, are one of the hallmarks of frustrated magnetism. We have shown how an extremely robust half-magnetization plateau can arise from coupling between spin and lattice degrees of freedom in a pyrochlore antiferromagnet, and developed a detailed symmetry analysis of the simplest possible scenario for such a plateau state. Our theory explains the magnetization curve in $CdCr_2O_4$ and $HgCr_2O_4$ spinel oxides, where a robust half magnetization plateau has been observed.

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The antiferromagnetic Ising model on a checkerboard lattice has an ice-like ground state manifold with extensive degeneracy and, to leading order in J_{xy}, deconfined spinon excitations. We explored the role of cyclic exchange arising at order J_{xy}^2/J_z on the ice states and their associated spinon excitations. By mapping the original problem onto an equivalent quantum six-vertex model, we identified three different phases as a function of the chemical potential for flippable plaquettes: a phase with long range Néel order and confined spinon excitations, a nonmagnetic state of resonating square plaquettes, and a quasicollinear phase with gapped but deconfined spinon excitations.

Other problems. — We presented a theory of cultural evolution based upon a renormalization group scheme. We consider rational but cognitively limited agents who optimize their decision making process by iteratively updating and refining the mental representation of their natural and social environment. These representations are built around the most important degrees of freedom of their world. Cultural coherence among agents is defined as the overlap of mental representations and is characterized using an adequate order parameter. As the importance of social interactions increases or agents become more intelligent, we observe and quantify a series of dynamic phase transitions by which cultural coherence advances in the society. A similar phase transition may explain the so-called "cultural explosion" in human evolution some 50,000 years ago.

We examined a previous statement that the orbital Kondo effect disappears when more and more orbital states of heavy particle are taken into consideration in the dynamic electron scattering, i.e., when the two-level system (TLS) is generalized to many-level system. A complete set of orbital states really cancel the logarithmic corrections at high temperatures but the high-energy states freeze out succesively when reaching the relevant temperature range. The aim is to find a realistic TLS to handle this freezing out in the calculations.

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Grants

OTKA T 043330	Theoretical study of strongly correlated low-dimensional systems (J. Sólyom, 2003-2006)
OTKA F 046356	Development and application of the momentum-space density-matrix renormalization group method for fermionic systems (Ö. Legeza, 2004-2007)
OTKA T 047003	Statistical physics of evolutionary games (Participant: G. Fáth, 2004-2007)

Publications

Articles

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

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A.3. Carmelo* JMP, Penc K, Martelo* LM, Sacramento* PD, Dos Santos* JMBL, Claessen* R, Sing* M, Schwingenschlogl* U; One-electron singular branch lines of the Hubbard chain; *Europhys Lett*; **67**, 233-239, 2004

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A.6. Shannon* N; Misguich* G; Penc K; Cyclic exchange, isolated states, and spinon deconfinement in an XXZ Heisenberg model on the checkerboard lattice; *Phys Rev B*; **69**, 220403(R)/1-4, 2004

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A.10. Legeza Ö, Sólyom J; Quantum data compression, quantum information generation, and the density-matrix renormalization group method; *Phys Rev B*; **70**, 205118/1-7, 2004

A.11. Fáth G, Sarvary* M; A renormalization group theory of cultural evolution; *Physica A*; accepted for publication

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

B. COMPLEX SYSTEMS

F. Iglói, N. Menyhárd, A. Sütő, P. Szépfalusy

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

Phase transitions and critical behaviour. — We have studied by extensive density matrix renormalization group (DMRG) calculations spin S = 1/2 and S = 3/2 disordered antiferromagnetic Heisenberg chains, which show a rather distinct behavior in the two cases. While at sufficiently strong disorder both systems are in a random singlet phase, we show that weak disorder is an irrelevant perturbation for the S = 3/2 chain, contrary to what expected from a naive application of the Harris criterion. The observed irrelevance is attributed to the presence of a new correlation length due to enhanced end-to-end correlations. This phenomenon is expected to occur for all half-integer S > 1/2 chains. A possible phase diagram of the chain for generic S is also discussed.

We have studied nonequilibrium dynamical properties at a free surface after the system is quenched from the high-temperature phase into the critical point. We have shown that if the spatial surface correlations decay sufficiently rapidly the surface magnetization and/or the surface manifold autocorrelations has a qualitatively different universal short time behavior than the same quantities in the bulk. At a free surface cluster dissolution may take place instead of domain growth yielding stationary dynamical correlations that decay in a stretched exponential form. This phenomenon takes place in the three-dimensional Ising model and should be observable in real ferromagnets.

An investigation has been started to explore the effect of quenched disorder in non-equilibrium systems showing compact directed percolation and parity conserving type phase transitions in one-dimension. The first results of large scale computer simulations in spin- and cellular automata systems point to no dramatic changes like those known for directed percolation-type phase transitions

Quantum systems. — For a system of atoms with spin s obeying Fermi statistics, it has been shown that the ground state consists of clusters of (2s+1) particles as a generalization of Cooper pairing for s=1/2.

Properties of spinor Bose gases (with spin 1) have been investigated in the presence of an external magnetic field. A magnetic transition prior to the Bose-Einstein condensation has been found.

In the chiral quark-meson model the phase diagram has been determined by changing the temperature and the chemical potential of the fermion gas. In particular the location of the critical end point (existing in the presence of explicite symmetry breaking) has been determined and its properties have been clarified.

Correlation inequalities for occupation number operators in noninteracting Bose gases have been derived. A study of normal and generalized Bose-Einstein condensation in trapped Bose gases has been performed with a special care on one-dimensional examples.

Quantum dynamical lower bounds have been obtained for a number of discrete one-dimensional Schrödinger operators by using power-law bounds on transfer matrices.

Other researches. — An *ab initio* method of phase retrieval in crystallography has been elaborated.

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Grants and international cooperations

OTKA T046129 Dynamics of phase transitions and symmetry breaking phases (P. Szépfalusy, 2004-2006)

OTKA T042914 Mathematical study of interacting Fermi and Bose systems (A. Sütő, 2003-2005)

OTKA T034183 Disordered quantum spin systems (F. Iglói, 2001-2004)

DAAD-MÖB 4/2004 Statistical physics of nonequilibrium and disordered systems (F. Iglói, 2004-2005)

TÉT F-17/03 (Hungarian-French) Statistical physics of disordered systems (F. Iglói, 2004-2005)

Publications

Articles

B.1. Carlon* E, Lajkó* P, Rieger* H, Iglói F; Disorder induced phases in higher spin antiferromagnetic Heisenberg chains; *Phys Rev B*; **69**, 144416/1-5, 2004

B.2. Pleimling* M, Iglói F; Out-of-equilibrium dynamics at surfaces: Cluster dissolution and non-algebraic correlations; *Phys Rev Lett*; **92**, 145701/1-4, 2004

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B.6. Pleimling* M, Bagaméry* FÁ, Turban* L, Iglói F; Logarithmic corrections in the two-dimensional Ising model in a random surface field; *J Phys A*; **37**, 8001-8009, 2004

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B.8. Jakovác* A, Patkós* A, Szép* Zs, Szépfalusy P; T-m phase diagram of the chiral quark model from a large flavor number expansion threshold; *Phys Lett B*; **582**, 179-186, 2004

B.9. Jakovác* A, Patkós* A, Szép* Zs, Szépfalusy P; Analytic determination of the T-m phase diagram of the chiral quark model; *Heavy Ion Physics*; **19/1**, 1-8, 2004

B.10. Sütő A; Correlation inequalities for noninteracting Bose gases; *J Phys A*: Math Gen; **37**, 615-621, 2004

B.11. Sütő A; Normal and generalized Bose-Einstein condensation in traps: One dimensional examples; *J Stat Phys*; **117**, 301-341, 2004

B.12. Damanik* D, Sütő A, Tcheremchantsev* S; Power-law bounds on transfer matrices and quantum dynamics in one dimension II.; *J Funct Anal*; **216**, 362-387, 2004

See also: E.4., E.15.

C. ELECTRONIC STATES IN SOLIDS

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

Within the frame of a bilateral cooperation with the Turku University we have developed an efficient procedure to calculate **surface segregation** profiles of substitutionally disordered binary alloys. We have shown that a simple thermodynamical model with realistic atomic configurations at the surface region combined with the total energies obtained from exact muffin-tin orbitals calculations leads to accurate surface segregation profiles. The calculated surface segregation energies in random alloys show significant dependence on the local environment of atoms involved in the segregation process. As an example the PdAg(111) surface was considered.

Using the density functional theory, formulated within the framework of the exact muffin-tin orbitals method, 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. In cooperation with the University of Uppsala we have started to investigate the effect of layer relaxation on the surface stress for different surface facets as well.

We performed calculations for electronic and magnetic properties of surface states confined by a circular **quantum corral** built of magnetic ad atoms (Fe) on a Cu(111) surface. The calculations are performed fully relativistically using the embedding technique within the Korringa-Kohn-Rostoker method. We showed the oscillations of charge and magnetization densities and the possibility of the appearance of spin-polarized states. In order to classify the peaks in the calculated density of states with orbital quantum numbers we also analyzed the problem in terms of a simple quantum mechanical circular well model. We used this model to estimate the behavior of the magnetization and energy with respect to the radius of the circular corral and found that there are ranges of radii where the spin-down state is occupied but the corresponding spin-up one is empty and therefore the surface states hold a finite magnetic moment.

We also investigated the experimentally observed canted moments in Co **nanowires** at Pt substrate step edges. For this reason we developed a new first principles spin-dynamics code which could calculate the orientation of the atomic magnetization. We found that the magnetization in the Co/Pt(111) step edge system tilts 42 degrees towards the step edge in excellent agreement with experiment (43 degrees). We were able to analyze the details of this magnetization based on the simulation. We also found that typical blocking temperatures may be smaller than previous theories predicted.

Motivated by the absence of cooperative Jahn-Teller effect and of **magnetic ordering** in $LiNiO_2$, a layered oxide with triangular planes, we studied a general spin-orbital model on the triangular lattice. A mean-field approach reveals the presence of several singlet phases between the SU(4) symmetric point and a ferromagnetic phase, a conclusion supported by exact diagonalizations of finite clusters. We argue that one of the phases, characterized by a large number of low-lying singlets associated to dimer coverings of the triangular lattice,

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

could explain the properties of $LiNiO_2$, while a ferro-orbital phase that lies nearby in parameter space leads to a new prediction for the magnetic properties of $NaNiO_2$.

The correlated 3d sulphide $BaVS_3$ is a most interesting compound because of the apparent **coexistence of one-dimensional and three-dimensional properties**. Our ARPES experiments explain this puzzle and shed new light on its electronic structure. High-resolution angle-resolved photoemission measurements in a 4 eV wide range below the Fermi level explored the coexistence of weakly correlated a_{1g} wide-band and strongly correlated eg narrow-band d-electrons that is responsible for the complicated behavior of this material. The most relevant result is the evidence for $a_{1g\text{-}eg}$ inter-band nesting condition.

Recent experiments on URu_2Si_2 show that the low-pressure hidden order is non-magnetic but it breaks time reversal invariance. Restricting our attention to local order parameters of 5f2 shells, we found that the best candidate for hidden order is staggered order of either T^z(beta) or T^{xyz} octupoles. Group theoretical arguments for the effect of symmetry-lowering perturbations (magnetic field, mechanical stress) predict behavior in good overall agreement with observations. We illustrated our general arguments on the example of a five-state crystal field model which differs in several details from models discussed in the literature. The general appearance of the mean field phase diagram agrees with the experimental results. In particular, we find that a) at zero magnetic field, there is a first-order phase boundary between octupolar order and large-moment antiferromagnetism with increasing hydrostatic pressure; b) arbitrarily weak uniaxial pressure induces staggered magnetic moments in the octupolar phase; and c) a new phase with different symmetry appears at large magnetic fields.

In the normal state of the **high-temperature superconductor cuprates**, using the experimental results of the photoemission measurement, we calculated both the Raman spectra and the infrared conductivity. Starting from a one band model in the random phase approximation, we assumed that the electron self energy can be approximated by the marginal Fermi liquid picture. The calculated spectra, at least in the low energy region are in very good agreement with the experimental results in a wide doping and temperature range. In the high energy region the one band approximation fails, and the contributions from the interband transitions play the dominant role.

We have investigated some special transport properties of **unconventional density waves** (UDW) in quasi one dimensional systems. These include the angular dependent magnetoresistance (ADMR), the magnetothermopower (MTP) and the Nernst effect. Comparison with MTP and Nernst data on the organic conductor α-$(ET)_2$ yielded quantitative agreement, confirming that the low temperature phase of this salt is a UDW. Our results on ADMR turned out to be applicable to another Bechgaard salt, $(TMTSF)_2PF_6$ as well. Predictions for the Raman spectra in UDW has also been given within our model.

We have calculated the frequency dependent conductivity of the unconventional superconductor Sr_2RuO_4, assuming *f-wave* symmetry of the order parameter. Based on our ADMR results, we proposed the appearance of a d-UDW in the pseudogap phase of underdoped high-T_c cuprates. Our findings reproduce the experimental results on optical dichroism as well.

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Grants and international cooperations

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

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

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

TÉT SF-15/03 (Hungarian-Finnish) Quantummechanical modelling of structural, electronic and magnetic properties of alloy surfaces (J. Kollár, 2004-2005)

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

Publications

Articles

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C.2. Kollár J, Vitos L, Osorio-Guillén* JM, Ahuja* R; Calculation of surface stress for fcc transition metals; *Phys. Rev B*; **68**, 245417, 2003

C.3. Pella* S, Faulkner* JS, Stocks* GM, B. Újfalussy; Electronic structure calculations on alloys using the Polymorphous Coherent-Potential Approximation; *Phys Rev B*; **70**, 064203/1-5, 2004

C.4. Eisenbach* M, Stocks* GM, ÚjfalussyB; Magnetic structure of iron inclusions in copper; *J Appl Phys*; **95**, 6684-6686, 2004

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C.6. Vernay* F, Penc K, Fazekas P, and Mila* F; Orbital degeneracy as a source of frustration in $LiNiO_2$; *Phys Rev B*; **70**, 014428/1-17, 2004

C.7. Dóra* B, Maki* K, Ványolos* A, Virosztek A; Magnetothermopower in unconventional density waves; *Synth Metals*; **141**, 103-107, 2004

C.8. Dóra* B, Maki* K, Virosztek A, Ványolos* A; Magnetothermopower in unconventional charge density wave ground state of α-$(BEDT\text{-}TTF)_2KHg(SCN)_4$; *J Physique IV*; **114**, 301-303, 2004

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C.10. Virosztek A, Dóra* B, Maki* K; Optical conductivity of the triplet superconductor Sr_2RuO_4; *Physica*; **C408-410**, 686-687, 2004

C.11. Dóra* B, Maki* K, Virosztek A, Ványolos* A; Unconventional spin density wave in Bechgaard salt $(TMTSF)_2PF_6$; *Europhys Lett*; **67**, 1024-1030, 2004

C.12. Lazarovits* B, Újfalussy B, Szunyogh* L, Győrffy* BL, Weinberger* P; Magnetic properties of quantum corrals from 'first principles' calculations; *J Phys: Condens Matter*; accepted for publication

C.13. Lazarovits* B, Újfalussy B, Szunyogh* L, Stocks* GM, Weinberger* P; Ab initio study of canted magnetism of finite metallic chains at surfaces; *J Phys: Condens Matter*; accepted for publication

C.14. Újfalussy B, Stocks* GM, Szunyogh* L, Lazarovits* B; Ab initio spin-dynamics studies of small metallic particles on surfaces; *J Magn Magn Mater*; accepted for publication

C.15. Sönderlind* P, Landa* A, Sadigh* B, Vitos L, Ruban* A; First-principles elastic constants and phonons of δ-Pu; *Phys Rev B*; accepted for publication

C.16. Landa* A, Sönderlind* P, Ruban* A, Vitos L, Pourovskii* LV; First-principles phase diagram for Ce-Th system; *Phys Rev B*; accepted for publication, (2004)

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C.18. Ropo* M, Kokko* K, Vitos L, Kollár J; Segregation at the PdAg(111) surface: Electronic structure calculations; *Phys Rev B*; accepted for publication

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C.19. Maki* K, Dóra* B, Virosztek A; Aspects of unconventional density waves. In: *AIP Conf. Proc.*; **695**, 10-20, 2003

C.20. Ványolos* A, Virosztek A; Electronic Raman scattering in density waves; In: *AIP Conf. Proc.*; **715**, 245-254, 2004

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C.23. Canning* A, Újfalussy* B, Schulthess* T, Zhang* X-G; Multi-teraflops studies of the magnetic structure of FeMn alloys and interfaces; In: *Parallel and Distributed Scientific and Engineering Computing: Practice and Experience*; Eds: Y. Pan and L.T. Yang, Nova Science, 2004

See also: A.5.

D. NON-EQUILIBRIUM ALLOYS

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

Rigid magnetic foam-like behaviour in ball-milled FeAl. — After ball-milling nonmagnetic FeAl a grain structure resembling to a rigid magnetic foam is indicated by Mössbauer spectroscopy. It consists of nanosize nonmagnetic grains with ferromagnetic boundaries formed by about two atomic layers of Fe. The magnetic behaviour is uncommon: (i) the transition to the paramagnetic state is *glass-like* and magnetic relaxation sets in at low temperatures; (ii) the *magnitude* of the local Fe magnetic moments decreases *linearly* with temperature; (iii) in high fields a *strongly anisotropic* ferromagnetic behaviour is observed.

FeAl crystallizes to a CsCl-type (B2) crystal structure, in which each Fe atom has 8 Al nearest and 6 Fe next nearest neighbors. While it is nonmagnetic, cold-working restores magnetism due to the formation of antiphase boundaries. The partial replacement of an Al plane by an Fe plane creates magnetic moments on the formerly nonmagnetic iron atoms since iron atoms having at least four Fe nearest neighbors are magnetic. (The number of the nearest Fe neighbors reaches 4 Fe along a two iron atom thick boundary). Ball-milling of the FeAl ingot leads to the gradual disordering of the ordered B2 structure as shown by the Mössbauer spectra in Fig. 1. The single line corresponding to the ordered nonmagnetic phase disappears for the 100 h ball-milled sample but the crystal structure remains. Also an increasing amount of broad, magnetic component appears that has a double-peaked hyperfine field (hf) distribution: the shadowed high-field part with the p_M spectral weight is due to the magnetic Fe atoms and the low-field part is due to the nonmagnetic Fe atoms with magnetic neighbors.

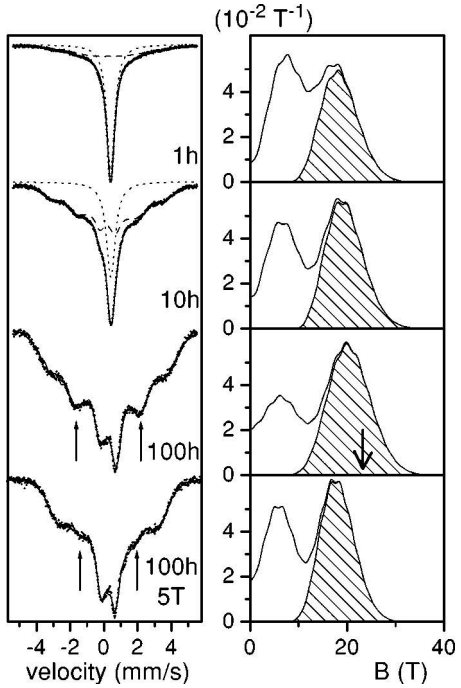

Fig. 1. 4.2 K Mössbauer spectra of FeAl ball-milled for different times. Full, broken, and dotted lines are fitted curves of the full spectra and the magnetic and the paramagnetic components, respectively. In the hyperfine field distributions fitted to the magnetic components shading and an arrow marks the hyperfine field of Fe atoms with localized moments and that of Fe atoms with 4 Al-4 Fe nearest neighbours in Fe_3Al, respectively. The positions of the second and fifth lines for the high field peak in the spectra of the 100 h sample in 0 T and 5 T field are marked as well.

The magnetic iron atoms mostly belong to the grain boundaries in the ball-milled samples. p_M correlates well with the inverse of the average grain size (Fig. 2). The slope of this correlation is proportional to the thickness of the boundary region, d. The proportionality coefficient is dependent on the shape of the grains; in the simplest cases (sphere or cube) it is $6d$. In our case this relation gives $d \approx 0.8$ nm for the average thickness of the grain boundaries. It may be somewhat overestimated due to the well-known bias of x-ray diffraction by the contribution of larger grains and to some disorder within the grains.

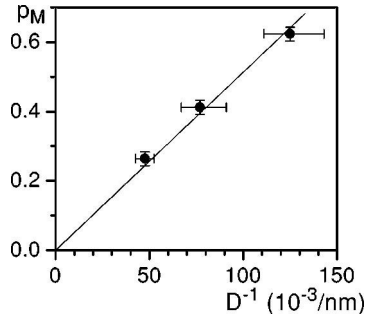

Fig. 2. The fraction of magnetic Fe atoms, p_M, in the ball-milled FeAl alloys as a function of the inverse grain size, D^{-1}. The proportionality is shown by the full line

Figure 3 shows the results of the SQUID measurements. In small magnetic fields the magnetization shows a broad peak as a function of temperature both in field- and in zero-field-cooled states. This feature resembles the freezing of a spin glass. However, the zero-field Mössbauer measurements show no magnetic character around the temperature of the peaks. Indeed, the Mössbauer spectra show no well-defined transition from the magnetic to the nonmagnetic state: superparamagnetic relaxation starts already at 12 K and 50 K for the 1 h and 100 h ball-milled samples, respectively. It means that already small magnetic fields influence greatly the magnetic state of these alloys. However, the magnetization cannot be saturated even in 5 T (Fig. 3(b)), which is caused by strong magnetic anisotropy as the presence of the 2-5 lines of the Mössbauer spectrum indicates in Fig. 1. If a linear extrapolation were justified, at least 14 T and 18 T would be necessary to reach saturation for the 100 h and 10 h ball-milled samples, respectively. The thermomagnetic curves in 5 T show complex temperature dependences and no distinct features (Fig. 3(c)).

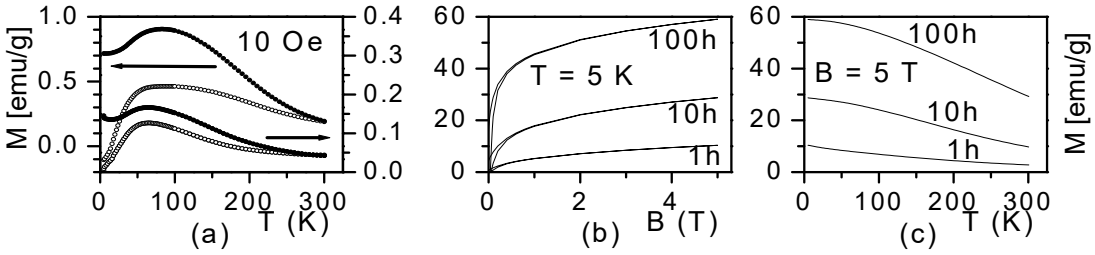

Fig. 3. Low-field behavior of the 10 h (right) and 100 h (left) ball-milled FeAl alloys in zero-field (circles) and in field-cooled (dots) states (a), the magnetization as a function of external field at 5K (b), and temperature dependence in 5 T external field (c).

Fe/Ag granular multilayers and heterostructures. — Multilayer deposition technique offers the possibility to prepare magnetically heterogeneous granular systems with controlled size and spacing of the magnetic elements. The study of such systems is important both for technical applications and for our understanding of the nature of interactions among the magnetic elements in nanoscale structures. ^{57}Fe(x)/Ag(2.6 nm) granular multilayers and heterostructures containing both granular (0.2 nm nominal Fe layer thickness) and continuous Fe layers (1.5 nm nominal layer thickness) have been prepared by molecular beam evaporation (MBE) at the Katholieke Universiteit in Leuven. The magnetic properties were examined by SQUID magnetometry and Mössbauer spectroscopy. The magnetoresistance was measured in parallel and transversal magnetic fields up to 12 T at the Budapest University of Technology and Economics. The granular layers show superparamagnetic properties above 38K. It was shown that the average blocking temperature and the low temperature out of plane magnetic alignment of the granular layers are not altered by continuous Fe layers (3:1 ratio of the granular and the continuous layers), either they are interleaved among the granular layers or placed separately at the bottom as a

multilayer buffer. On the other hand the temperature dependence of the large field magnetoresistance was found to be significantly different for the separated and the interleaved samples. These results support the view that besides the size of the superparamagnetic grains the induced spin asymmetry of the conduction electrons plays an important role in the magnetoresistance of heterogeneous systems.

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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, 2000-2004)
OTKA T034602	Magnetic properties of multilayers (J. Balogh, 2001-2004)
OTKA T038383	Interaction of superparamagnetic clusters (L.F. Kiss, 2002-2005)
OTKA T046795	Superferromagnetism in nanostructures (I. Vincze, 2004-2007)

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Articles

D.1. 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*; **A375-377**, 219-222, 2004

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See also H.3., H.4., H.5., H.11.

E. X-RAY DIFFRACTION

G. Faigel, F. Borondics[#], G. Bortel, L. Gránásy, A. Jánossy[+], Z. Jurek, K. Kamarás, G. Klupp[#], É. Kováts[#], G. Oszlányi, S. Pekker, T. Pusztai, Gy. Tóth[#], 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. In the last few years an interesting area of research is the topochemistry of fullerenes and related materials. In connection with this, we study the polymerization of fullerenes and their derivatives, and the cycloadditions of fullerene inclusion compounds. Our studies are mainly experimental such as preparation techniques, HPLC separation, x-ray diffraction and spectroscopic methods but in a smaller extent we also perform quantum chemical calculations. Further we have prepared new materials: host-guest compounds of fullerenes with various reactive guest molecules, which can be the precursors of further copolymerization reactions.

Similarly to the fullerene molecules, carbon nanotubes are also exclusively built from carbon atoms. An important line of research connected to nanotubes is their functionalization. We have worked out a new reductive functionalization method and prepared various alkylated and arylated derivatives. Further, we have studied the optical properties of pristine and functionalized carbon nanotubes by wide-range optical spectroscopy (far-infrared through ultraviolet) and Raman spectroscopy. We have developed methods for preparing thin carbon nanotube layers on various substrates and also freestanding thin films. On these samples, we studied the effects of ionic doping and chemical functionalization on the optical spectra.

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 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 asses 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. In previous years we developed a model, which describes the behavior of a cluster of carbon atoms in the x-ray FEL pulse. This model was extended to the description of multicomponent system. It was found that the clusters explode. The dynamics of the Coulomb explosions for various systems were analysed. We showed that useful structural data could only be collected in the first part of a pulse. Using a special reconstructing algorithm we could invert the continuous elastic scattering pattern to real space structure. Beside the feasibility of structure determination our calculations give an insight to the physics of cluster explosion.

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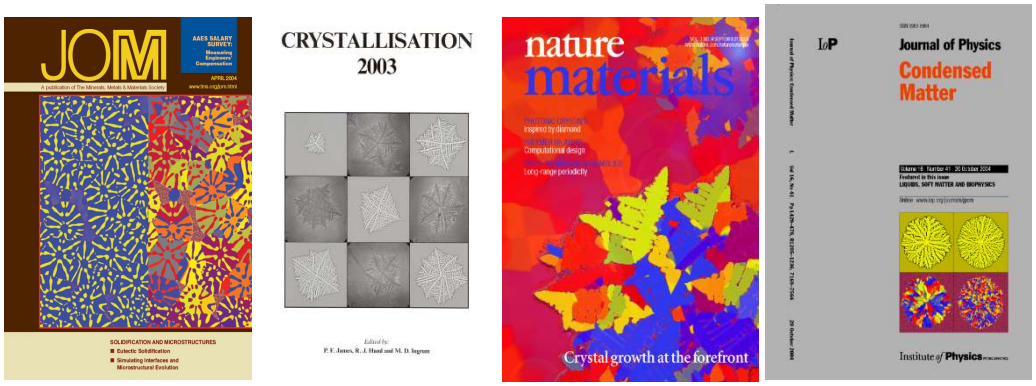
Ab initio structure solution. — Inspired by existing methods of image reconstruction, we started the development of new structure solution methods in x-ray crystallography. Our first result is an amazingly simple iterative algorithm, named charge flipping. It works on high-resolution single crystal data, in the manner of Fourier recycling. The real space modification simply changes the sign of charge density below a threshold, while in reciprocal space observed structure factor moduli are combined with the calculated phases. The method is truly ab initio, the knowledge of chemical composition or even atom types are not required. Symmetry information is not used either, the correct space group can be deduced from the electron density of the solution.

Theory of phase transformations. — Eutectic solidification with fixed orientational relationship between the solid phases has been modeled using the phase field theory [Fig. 1(a)]. We presented a phase field theory for the nucleation and growth of one and two phase crystals solidifying with different crystallographic orientations in binary alloys. The accuracy of the model has been tested for crystal nucleation in single component systems. It is shown that without adjustable parameters the height of the nucleation barrier is predicted with reasonable accuracy. The kinetics of primary solidification is investigated as a function of model parameters under equiaxial conditions. We studied the formation of complex polycrystalline growth morphologies [disordered dendrites, spherulites and fractal-like aggregates, see Figs. 1(b)-(d)]. Via extensive modeling, we identified the main mechanisms that govern the formation of complex polycrystalline patterns: diffusional instabilities, growth front nucleation due to foreign particles or quenched-in orientational defects, and crystallographic branching with fixed misorientation. It has been found that static heterogeneities (foreign particles) and dynamics heterogeneities (quenched-in orientational disorder) lead to similar randomized growth morphologies. We have extended our phase field approach to the formation of CO_2 hydrate in aqueous solutions, and predicted the growth and nucleation rates.



(a) (b) (c) (d)

Fig. 1. Front covers based on our phase field simulations:
(a) JOM ***56****, N° 4, 2004;*
(b) Physical Chemistry of Glasses ***45****, 2004;*
(c) Nature Materials, ***3****, N° 9, 2004;*
(d) Journal of Physics: Condensed Matter ***16****, N° 41, 2004*

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Grants and international cooperations

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

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

OTKA T 034198 Temperature and pressure dependent optical studies on 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)

ESA PECS 98005 Phase field modeling of magnetic and composite materials (L. Gránásy, 2004–2006)

EU FP6 –500635-8 IMPRESS Intermetallic Materials Processing in Relation to Earth and Space Solidification (L. Gránásy, 2004–2009)

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Articles

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E5. Lewis* D, Pusztai T, Gránásy L, Warren* J, Boettinger* W; Phase field models for eutectic solidification; *JOM*; **56**, 34-39, 2004

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E.19. Gránásy L, Pusztai T, Tegze G, Kuznetsova* T, Kvamme* B; Towards a full dynamic model of CO_2 hydrate formation in aqueous solutions: Phase field theory of nucleation and growth; In: *Advances in Research of Gas Hydrates;* Taylor CE, Kwan JT (eds.), Springer, Berlin; accepted for publication

E.20. Gránásy L, Pusztai T, Börzsönyi T, James* PF; Continuum models for crystal nucleation in undercooled melts and glasses; In: *Nucleation Control;* Greenwood GW, Greer AL, Herlach DM, Kelton KF (eds.), Cambridge Univ. Press, Cambridge; accepted for publication

See also: D.13.

F. ELECTRON CRYSTALS

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

Nuclear magnetic resonance in fullerides. — A long standing problem in the nuclear magnetic resonance (NMR) spectroscopy of the alkali fullerides A_3C_{60} (A = Rb or K) is the splitting of the NMR line of the alkaline nuclei of tetrahedral C_{60} coordination. To gain new insight to this intriguing problem, we have investigated the ^{23}Na nuclear magnetic resonance (NMR) spectrum and spin-spin relaxation time in Na_2CsC_{60} in the temperature range of 10 to 325 K. We find a single line above about 170 K but two lines (denoted by T and T', respectively) are present below this temperature. The closely similar temperature dependences of the spin-spin relaxation rates of the two lines as well as the temperature dependence of the first moment of the spectrum both below and above of the temperature of line splitting indicate a chemical exchange between these lines. Moreover, a correlation is found between the temperature dependence of the ^{13}C line width and the temperature dependence of the intensity of the T' line (the less intense line of the two). These findings lead us to suggest that the difference between the sodium sites giving rise to the T and T' lines lies in different angular orientations of the fullerene ions surrounding these sites. Based on x-ray structural results, we make detailed propositions about the C_{60} orientations around the T and T' sites. These results suggest a similar origin of the T–T' splitting in A_3C_{60}, where structural data are less accurate because of the merohedral disorder of C_{60} molecules in this class of materials.

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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[1] principal investigator: G. Kriza, 2002-2004)

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

Publications

Articles

F.1 Matus P, Alloul* H, Kriza G, Brouet* V, Singer* PM, Garaj* S, Forró* L; NMR evidence for C_{60} configurational fluctuations around Na sites in Na_2CsC_{60}; *J Superconductivity;* accepted for publication

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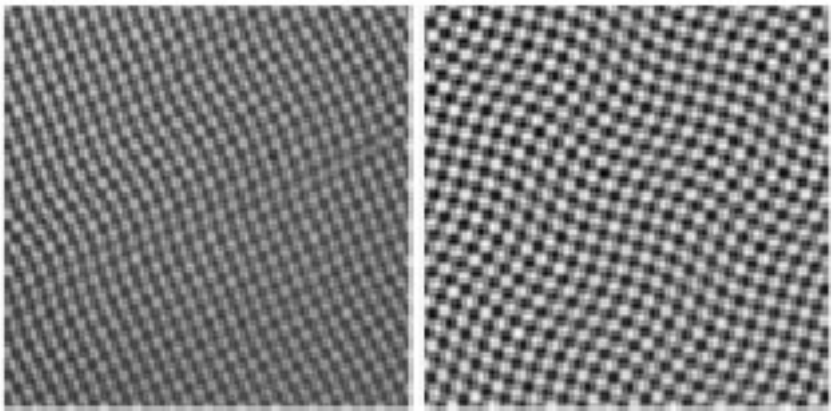
See also: E.14.

G. LIQUID CRYSTALS

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

Experimental **electroconvection** has been studied on four homologues with various magnitude and sign of the conductivity anisotropy (σ_a). The homologue with $\sigma_a>0$ follows the predictions of the standard theoretical model while the one with $\sigma_a<0$ shows a stripe pattern mainly parallel with the initial director, not described by the Carr-Helfrich (standard) mechanism. The remaining two homologues change sign of σ_a with temperature thus perform a crossover from the standard to non-standard electroconvection. Both types of patterns have been experimentally characterized and compared.

A new variant of electroconvection in a homeotropically aligned nematic has been studied. The novelty of the system is a direct transition to roll- and square-type patterns controlled by the frequency of the applied voltage with a rich crossover scenario and strong influence of the zigzag instability even at onset. From the weakly nonlinear theory and simulations of an adapted Swift-Hohenberg model the essential features of the phase diagram has been understood. In particular a long-wave modulated quasiperiodic pattern with square symmetry has been found.



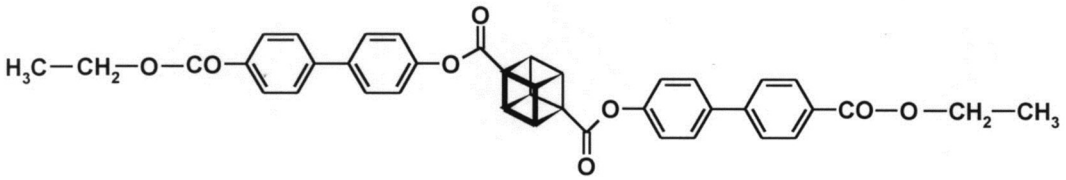
Long-wave modulated quasiperiodic square pattern in experiment and simulation

The distribution spectra of the fluctations in the amount of power injected into a liquid crystal undergoing electroconvective flow has been measured. The probability distribution functions (PDFs) of the fluctuations as well as the magnitude of the fluctuations have been determined in a wide range of imposed stress both for *unconfined* and *confined* flow geometries. These spectra were compared to those found in other systems held far from equilibrium. The PDF approaches the universal form via an interesting mechanism whereby the distribution's negative tail evolves towards a form in a different manner than the positive tail.

It has been shown that the direction of the **alignment** of liquid crystals on soft polymer surfaces can be altered by an external field. The relaxation kinetics of a twist deformation induced by a magnetic field has been determined measuring the rotation of light polarization. The relaxation times show a strong temperature dependence approaching the glass transition of the polymer. This behaviour has been explained using a model based on the mutual interaction of the liquid crystal and the polymer surface.

[#] *Ph.D. student*

New symmetrical esters of **cubane-1,4-dicarboxylic acid** have been prepared. These compounds have the bulky cubane skeleton as a central building block. Five classes of derivatives have been synthesized. The lower homologues of the alkoxyphenyl-ester series exhibited a nematic (N) phase. No mesophase was observed on the pentyl derivative, while the higher homologues showed smectic A (SmA) phase according to X-ray investigations. The (4-alkyl)phenyl- and chiral derivatives showed only a melting point. Also the double swallow tailed bis[4-(2,2-alkoxycarbonyl-vinyl)phenyl)]cubane-1,4-dicarboxylate derivatives exhibited no mesophase.



Bis[(4'-ethoxycarbonyl)-1,1'-biphenyl-4-yl]-cubane-1,4-dicarboxylate

Increasing the number of the aromatic rings up to two on both sides of the central cubane moiety, nematic and SmA phases appeared at higher temperature.

Miscibility studies have been carried out in order to investigate the effect of terminal chain length on the mesophase behaviour of cubane derivatives. In binary mixtures composed of homologues of alkoxyphenyl cubane esters the temperature range of the SmA phase of the individual compounds became wider and enantiotropic. Moreover an additional crystalline modification (Cr_2) was also detected. In all binary mixtures of the cubane derivatives investigated an enhanced ability of SmA mesophase formation was observed. When the alkoxyphenyl cubane ester (having no mesophase) was mixed with 8OCB, at 30wt% of the added component an enantiotropic N phase appeared, at 70 wt% additionally a SmA phase was observable during heating.

After the calamitic cubanes the first bent-core cubane derivatives have also been prepared. The monomers were polymerized forming the first banana-shaped polymeric cubane esters.

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Grants and international cooperations

COST D14 WG 015	Advanced Molecules and Macromolecules Containing Banana-Shaped Mesogens for Photonic Materials (K. Fodor-Csorba, 2002-2005)
OTKA T-031808	Convective and interfacial instabilities in liquid crystals. (Á. Buka, 2000-2004)

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, 2000-2004)

OTKA T037275 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, 2004-2006)

MTA-CAS (Hungarian-Chinese bilateral) Physical and chemical study of liquid crystals. (N. Éber, 2004-2006)

MTA-SASA (Hungarian-Serbian bilateral) Structure and physical study of liquid crystals. (N. Éber, 2004-2006)

MTA-ASCR (Hungarian-Czech bilateral) Synthesis and study of ferroelectric liquid crystals leading to preparation of mixtures with defined properties. (K. Fodor-Csorba, 2004-2006)

MTA-CNR (Hungarian-Italian bilateral) New banana-shaped monomers and their polymer derivatives. (K. Fodor-Csorba, 2004-2006)

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)

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

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

COST D14 WG 0015 Advanced molecules and macromolecules containing banana-shaped mesogens for photonic materials. (K. Fodor-Csorba, 2002-2005)

56ÖU4 Austrian-Hungarian Action Foundation. Polymers made of banana-molecules – How to conserve unique properties. (K. Fodor-Csorba, 2004)

Long term visitors

— *David Statman*: Alleghiny College, Meadville, Pennsylvania, USA, 15 June-15 July, 2004, (host: I. Jánossy).

— *Elzbieta Kochowska*: The Henryk Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences, Cracow, Poland, 1 Januar- 4 October, 2004, (EU-RTN grant, host: Á. Buka).

— *Aude Cauquil-Vergnes*: University of Montpellier, Montpellier, France, 5 October – 31 December, 2004, (EU-RTN grant, host: Á. Buka).

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Articles

G.1. Tóth-Katona T, Gleeson* JT; Distribution of injected power fluctuation in electroconvection; *Phys Rev Lett*; **91**, 264501/1-4, 2003

G.2. Vajda A, Hamplova* V, Kaspar* M, Bubnov* A, Obadovic* DZ, Éber N, Fodor-Csorba K; Structure-property relationship studies on chiral lactic acid derivatives; *J of Research in Physics*; **29**, 107-113, 2003

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G.10. Jánossy I, Kósa* T; Gliding of liquid crystals on soft polymer surfaces; *Phys Rev E*; **70**, 052701/1-4, 2004

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G.12. Bényei* G, Slugovc* C, Trimmel* G, Vajda A, Pelzl* G, Jalsowsky I, Éber N, Fodor-Csorba K; New liquid crystalline cubane-1,4-dicarboxylicc acid derivatives. Structure and property study; *Liquid Crystals*; accepted for publication

G.13. Barmatov* E, Calucci* L, Catalano* D, Chiezzi* L, Fodor-Csorba K, Veracini* CA; ^{2}H-NMR and molecular ordering in the induced cholesteric chiral phases of acrylate-

metacrylate side chain liquid crystalline copolymers; *Mol Cryst Liquid Cryst*; accepted for publication

Conference proceeding

G.14. Bényei* G, Jalsovszky* I, Fodor-Csorba K; Structure-property relationship study on new cubane-1,4-dicarboxylic acid derivatives; In: *Proc. XV. CLC Conference 13-17 October 2003, Zakopane, Poland*; SPIE Proceedings; accepted for publication.

See also E.6., E.10., E.20.

H. METAL PHYSICS

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

NMR study of metal-hydrogen systems. — High-purity Pd metal and $Pd_{1-x}Ag_x$ (x = 0.1–0.35) alloys were charged with hydrogen from gas phase. Proton NMR free-induction decay and different echoes were measured down to 2.4 K. Samples of hydrogen content H/M = 0.04 to 0.7 were prepared and investigated. At very low temperatures (down to 2.4 K), inhomogeneous echoes ($\pi/2 - \tau - \pi/2(0°)$ – echo) were detected besides the commonly known solid echoes ($\pi/2 - \tau - \pi/2(90°)$ – echo) (Figure 1). The presence of the inhomogeneous echoes suggests that hydrogen in Pd and Pd-Ag alloys does not behave as a system of identical proton spins which are purely dipolar-coupled. An inhomogeneous contribution of unknown electronic origin explains the large second moments measured in samples of H/M < 0.06. We have found that the lattice-gas model used for the description of α-phase Pd and Pd-Ag hydrides is not able to explain this feature. The nature and behaviour of the detected echoes can be explained – as a working hypothesis – on the basis of three types of interactions. These are dipolar interaction between identical spins, dipolar interaction between non-identical spins and interaction of nuclear spins with a local field of electronic origin.

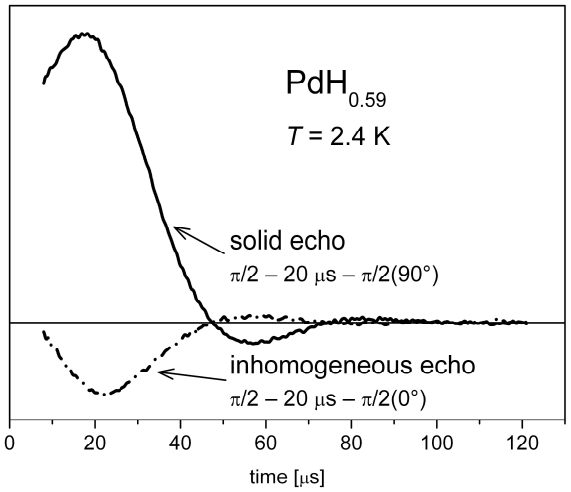

Figure 1. ^1H NMR echoes measured in $PdH_{0.59}$ at T = 2.4 K.

Looking for new fields of NMR research.

— *Hydrogenated carbon materials.* — Chemically hydrogenated single-wall carbon nanotube, graphite and fullerene samples were investigated by ^1H NMR. We have found that the chemically bound hydrogen forms two phases with respect to its mobility: a phase of "rigid lattice" and a mobile liquid-like phase.

— *Hydration of semi-structured proteins.* — ^1H NMR signals of physiological solutions of proteins were investigated (in cooperation with the Institute of Enzymology, Biological Research Center, HAS). The method provides data on both the amount and dynamics of bound water, the heterogeneity of which is unveiled by progressive freezing out. The technique enables the characterization of semi-structured proteins, showing their significantly larger hydration than globular proteins. The phases of ice protons, protein protons and (unfrozen) water protons are clearly separated in the free induction decay signal by virtue of large differences in the spin-spin relaxation rates. This enables specific recording of free induction decays that belong to the hydrate layer of proteins (Figure 2). The activation energy obtained for the dynamics of the most strongly bound part of the hydration shell is by 50% larger for semi-structured proteins than for a globular protein.

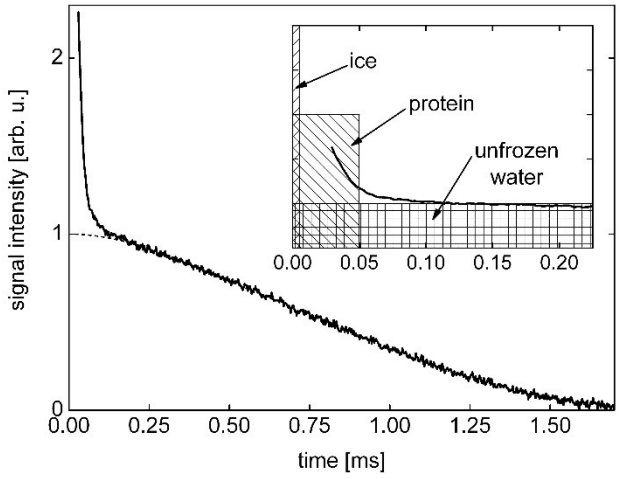

Figure 2. Illustration for the measurement of the fraction of unfrozen water component below 0 °C. The extrapolated signal intensity (dashed line) of the slowly decaying part of the FID signal was compared to the signal intensity measured above 0 °C to get the amount of unfrozen water. The inserted graph shows the typical time-spreads of FID signals produced by ice protons, protein protons and unfrozen water protons.

Electrolytic hydrogen charging/discharging of metals. — The resistivity was measured during the electrolytic hydrogenation of Pd metal foils. In the α-phase region, the resistivity increase was linear with the hydrogen content derived by assuming a current efficiency η = 1.100 % and the value of its slope was in good agreement with previously reported data. However, in the α+β mixed two-phase region, in order to get agreement with previous experiments in which the hydrogen content was determined directly after doping, we had to assume that there are some excess H atoms entering/leaving the Pd metal while charging/discharging hydrogen electrolytically. Formally, this excess amount of H atoms were quantified by introducing a current efficiency of η_a = 1.55 and η_d = 1.90 for the absorption and desorption process, respectively. These constants reflect the average number of extra protons which play an important role in the electolytic process as an inevitable concominant phenomenon.

GMR in electrodeposited multilayers. — It was shown that both the magnetization (M) and the magnetoresistance (MR) can be decomposed into a ferromagnetic (FM) and a superparamagnetic (SPM) term for multilayers with strongly non-saturating MR behaviour. The separation of the MR components was performed on the basis of a model elaborated for granular alloys with the simultaneous presence of both FM and SPM particles. This model predicts that conduction electron paths "FM region 1 → non-magnetic region → SPM region 2" (or in the reverse sequence) lead to a field (H) dependence of the MR that can be described by the relation MR(H) ∝ L(x) where L(x) is the Langevin function with x = μH/kT (μ: size of average SPM moment; T: temperature). It could be demonstrated that in multilayers the field dependence of the magnetoresistance can be described as MR(H) ∝ L(x) for magnetic fields beyond the saturation field (H_S) of the FM component. The typical size of the SPM regions deduced from the magnetic and MR data for the electrodeposited Co-Cu/Cu multilayers investigated was estimated to be about 6 nm x 6 nm x 3 nm in the form of separated islands. Fig. 3 shows an example for a multilayer in which the SPM term dominates. In another study, the results of potentiodynamic measurements and current transients recorded during pulse-plating of Co–Cu/Cu multilayers were compared. It was observed that the onset potential of Co dissolution as observed on the potentiodynamic curves depends on several experimental parameters such as sweep rate, cathodic limit, ion concentrations, pH and also on the number of cycles recorded. It was revealed that the potential at which Cu can be deposited after the deposition of the Co-rich layer *without the dissolution of Co* can be established only by the measurements of current transients during the potentiostatic Cu deposition pulse. Based on this new finding, Co-Cu/Cu multilayers

were prepared to completely avoid the dissoluton of Co during the Cu deposition pulse. This ensured that the actual amounts of metals deposited were equal to the nominal ones. Detailed studies were performed to establish the evolution of GMR with the "true" layer thicknesses in a wide thickness range of both the magnetic and non-magnetic layers. A GMR effect was observed in most samples and a maximum GMR of 10 % measured at 1 kOe could be achieved. No oscillatory GMR behaviour with increasing Cu layer thickness could be observed but rather a continuous evolution of the MR characteristics from anisotropic magnetoresistance (AMR) to GMR. This could be explained by the gradual increase of the Cu coverage on the Co-rich magnetic layer during each Cu pulse with increasing average Cu layer thickness. It was concluded that the Cu layer becomes continuous above about 2 nm thickness only. For 2.5 nm Cu layer thickness, the Co layer remained continuous down to 1.1 nm thickness. However, for 1.1 nm Cu layer thickness, the 1.1 nm thick Co layer was broken up into SPM islands. The evolution of the coercive force with layer thicknesses well corroborated the above picture. From these results, an asymmetry in the nucleation of Cu on Co and Co on Cu could be deduced in agreement with some previous reports on evaporated multilayers.

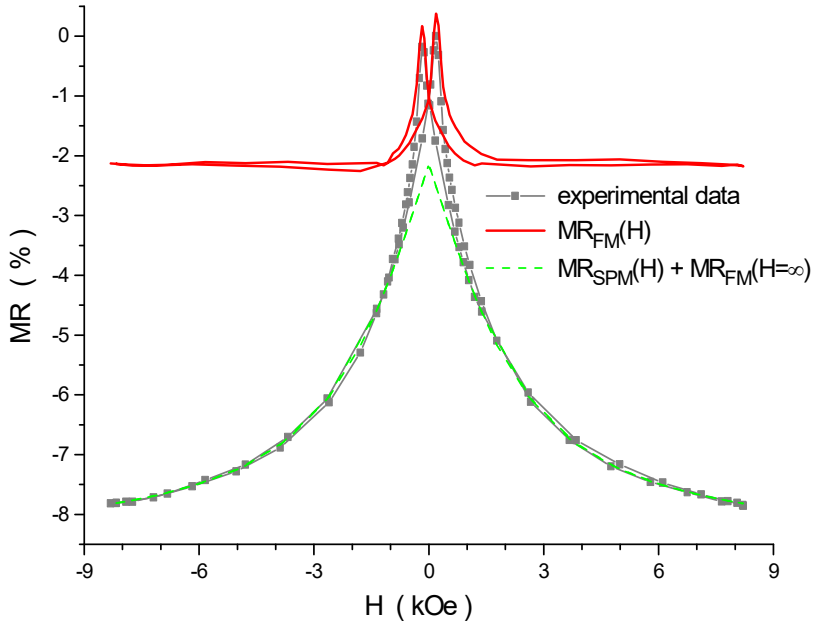

Figure 3. Decomposition of the room-temperature longitudinal magnetoresistance curves for an electrodeposited Co-Cu/Cu multilayer sample: measured data (symbols ■), decomposed FM (solid line) and SPM (dashed line) contributions to the observed magnetoresistance.

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Grants and international cooperations

OTKA F 032046 Preparation of metallic multilayers from compositionally modulated flowing electrolytes (L. Péter, 2000-2004)

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)

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

TéT TR-9/03 Hungarian -Turkish Bilateral Cooperation: Electrodeposition of nanostructured materials and their magnetic and magnetotransport characterization (I. Bakonyi, 2004-2005

Long term visitor

— M. Alper, University of Uludag, Bursa, Turkey, June 2004 (Hungarian-Turkish Bilateral Cooperation, host: I. Bakonyi).

— Q.X. Liu, Central Iron and Steel Research Institute (CISRI), Beijing, P.R. China, Jan. - Feb. 2004 (host: I. Bakonyi).

— I. Tapan, University of Uludag, Bursa, Turkey, July 2004 (Hungarian-Turkish Bilateral Cooperation, host: I. Bakonyi).

Publications

Articles

H.1. Cziráki* Á, Gemming* T, Weihnacht* V, Wetzig* K, Péter L, Pádár J, Bakonyi I, Tichy* G; Co-deposition, dissolution and replacement process during electrochemical deposition of Co/Cu multilayers; *Microscopy and Microanalysis;* **9**, Suppl 3, 244-245, 2003

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H.13. Bokor M, Csizmók* V, Bánki, Friedrich* P, Tompa* P, Tompa K; NMR relaxation studies on the hydrate layer of intrinsically unstructured proteins; *Biophysical Journal*; accepted for publication

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Others

H.17. Tompa K; Fizikus szemmel a 2003. évi élettani-orvostudományi Nobel-díjról (A physicist's view of the Nobel prize in physiology or medicine 2003; in Hungarian); *Szemészet;* **140**, 209-210, 2003

H.18. Tompa K; Vízmolekulák és élet: rádióhullámok az élőanyag-kutatásban (Water molecules and life: radio waves in research on living matter; in Hungarian); *Fizikai Szemle;* **53**, 247-254, 2003

H.19. Péter L; Néhány gondolat a természettudományi kutatások finanszírozásáról Magyarországon (Some remarks on the financing of scientific research in Hungary; in Hungarian); *Magyar Tudomány*; **101**, 784-786, 2004

H.20. Tompa K; 2003. évi élettani-orvostudományi Nobel-díj (The Nobel prize in physiology/medicine 2003; in Hungarian); *Természet Világa;* **135**, 2-4, 2004

H.21. Tompa K; A magyarországi NMR-kutatások kezdetei (The beginnings of NMR studies in Hungary; in Hungarian); *Magyar Kémiai Folyóirat;* **109-110**, 148-152, 2004

See also: E.14.

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. — We have prepared and characterized the structural and magnetic properties of various Co-doped FINEMET and HITPERM type alloys like

— $(Fe_{100-x}Co_x)_{73.5}Si_{13.5}B_9Nb_3Cu_1$ (Hitachi FINEMET)

— $(Fe_{100-x}Co_x)_{78}Si_9B_9Nb_3Cu_1$ (Yoshizawa FINEMET)

— $(Fe_{100-x}Co_x)_{84}Zr_{3.5}Nb_{3.5}B_8Cu_1$(HITPERM with Nb)

New amorphous compositions as precursor materials for nanocrystalline alloys have been developed:

— P-based: $Fe_{81}P_{13}Si_2Nb_3Cu_1$ and derivatives: $(Fe_{100-x}Co_x)_{81}P_{15-y}Si_yNb_3Cu_1$

— B-P-based (PYROPERM): $Fe_{84.5}Nb_5B_{8.5}P_2$ and derivatives:$(Fe_{100-x}Co_x)_{84.5}Nb_5B_{8.5}P_2$

New bulk amorphous alloy compositions with similar composition to the residual amorphous phase in the nanocrystalline alloys have been developed:

— for FINEMET: $Fe_{62}Nb_8B_{30}$ and derivatives: $(Fe_{100-x}Co_x)_{62}Nb_8B_{30}$

— for NANOPERM: $Fe_{67}Zr_3B_{30}$, $Fe_{67}Zr_8B_{25}$ and derivatives: $Fe_{67-x}Co_xZr_8B_{25}$

A combined electrochemical technique was developed to prepare iron layers with nanosized grains and subsequently Fe/Fe-oxide multilayers.

A furnace has been developed for heat treatment in magnetic field up to 1500 Oe at temperatures up to 800 °C. Toroidal samples with maximal outer diameter of 80 mm can be heat-treated to induce transversal anisotropy by magnetic field.

The switching field for a chain of monodomain particles has been studied by micromagnetic calculations in order to simulate the Jacobs-Bean model.

Magnetic domain imaging by SEM: noise analysis. — In order to improve the imaging of magnetic domains by SEM, we have carried out an analysis on how noise occurs and varies during data acquisition and data transformation. Estimating noise in digital images from a single recording of the scene is not always possible in an objective way since our perception of information and noise is very context sensitive. Generally speaking, it is impossible to completely separate information from noise in an objective way from any single image. It is the a priori knowledge that enables a human observer to distinguish information and noise better than an image processing system into which the sufficient amount of contextual knowledge is hard to incorporate. This is one of the main reasons why image processing solutions, to the present time, tend to remain within a well-defined, limited application range and it is difficult to generalize them and apply them in different environments. To overcome these difficulties, a method was elaborated for estimating the noise and signal level from noisy images if the scene can be recorded multiple - at least two - times and changes between the individual copies can be attributed solely to noise. We have regarded as noise only those factors which introduce random variations into a signal and can therefore be assessed and reduced by repeated acquisition. A defocused image clearly

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doesn't meet this criterion. We have even made a step further and considered everything that is constant in an image upon repeated acquisition as information.

Thermal expansion coefficient determination by temperature modulated dilatometry. — A technique applying modulated temperature in dilatometric analysis was developed. The major problems are knowing the temperature gradient within the sample and the sample-thermocouple path when the temperature is modulated. Knowing the sample temperature is crucial for proper interpretation of its thermal expansion. In order to determine the relationship between measured and expected temperatures, a multifrequency modulation program was applied and an electrical model of the measurement arrangement was used. The thermal expansion coefficients of a Cu-Zn alloy, nickel and iron around their critical temperatures were determined by using this procedure.

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Grants and internationa cooperations

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

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

OTKA T037643 Nanostructured functional coatings. (Research grant for the Chemical Research Center of HAS, participant: L.K. Varga, 2002-2005).

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, 2001-2004).

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 (Hungarian-Spanish Bilateral Science and Technology Cooperation) Preparation of new nanocomposite materials and their applications in materials engineering (L.K. Varga, 2001-2004)

TéT F-36/00 (Hungarian-French Bilateral Science and Technology Cooperation) Soft magnetic nanocomposites: preparation, characterization and

application in high-frequency power electronics (L.K. Varga, 2001-2004,)

HAS-SAS (Hungarian-Slovakian bilateral) Study of physical properties of special magnetic materials (L.K. Varga, 2001-2004)

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

Publications

Articles

I.1. Kamasa P, Myslinski* P, Pyda* M; Thermal expansion coefficient determination by temperature modulated dilatometry; *NATAS Notes* (North American Thermal Analysis Society); **35,** 17-21, 2003

I.2. Concustell* A, Révész* Á, Surinach* S, Varga LK, Heunen* G, Baró* MD; Microstructural evolution during decomposition and crystallization of the $Cu_{60}Zr_{20}Ti_{20}$ amorphous alloy; *J Mater Research*; **19**, 505-512, 2004

I.3. A. Concustell* A, Zielinska* M, Révész* Á, Varga LK, Suriñach* S, Baró* MD; Thermal characterization of $Cu_{60}Zr_xTi_{40-x}$ metallic glasses (x=15, 20, 22, 25, 30); *Intermetallics*; **12**, 1063-1067, 2004

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I.33. Varga LK, Mazaleyrat* F; Magnetic decoupling in soft magnetic nanocrystalline alloys; In: *Properties and Applications of Nanocrystalline Alloys from Amorphous Precursors (Proc. NATO ARW, Budmerice, Slovakia, 2003)*; Eds.: Idzikowski, B, Švec P, Miglierini M, NATO Science Series II, Kluwer, Dordrecht; accepted for publication

Book chapters

I.31. Konczos G; Gőzök leválasztása fizikai módszerekkel PVD (Physical vapour deposition, in Hungarian); In: Korszerű technológiák a felületi tulajdonságok

alakításában (Advanced technologies in development of surface properties); Ed.: Takács J, *Műegyetemi Kiadó, Budapest;* pp. 117-130, *2004*

I.32. Konczos G; Ionimplantáció (Ion implantation, in Hungarian); In: Korszerű technológiák a felületi tulajdonságok alakításában (Advanced technologies in development of surface properties); Ed.: Takács J, *Műegyetemi Kiadó, Budapest;* pp. 148-162, *2004*

See also H.1., H.3., H.7., H.11., H.14., J.10., S.24.

J. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

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The 10 MW Budapest Research Rector (BRR) and its experimental facilities on the KFKI campus 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 2004 by the local staff and in collaboration with national or foreign users coming from university, industrial or other research laboratories. We operate several cold and thermal neutron beam instruments: a small angle scattering (SANS) spectrometer, a reflectometer (REFL), a three axis spectrometer (TASC) and a cold neutron beam test facility as well as a thermal beam three axis spectrometer (TAST) and time-of-flight diffractometer (TOFD, under commissioning). 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 FZ Jülich, HMI Berlin, ISIS (UK) or LLB Saclay (France).

The scientific activity of our team is focused on neutron optics research, investigation of structure and dynamics of liquids, soft and solid matters as well as of materials with industrial relevance. A considerable effort of our team is also devoted to development of neutron scattering techniques.

Neutron optics. — We have continued to explore experimental possibilities of atomic resolution neutron holography. The realization of the so called internal source approach on a metalhydride sample was completed. The holographic image of a PdH single crystal was obtained. This experiment is our second successful demonstration of the capabilities of the atomic resolution neutron holography technique and the first step towards the dissemination of the holography method for the routine study of hydrogen containing materials.

Liquids. — In *aqueous solutions of polyfunctional alcohols*, similarly to solutions of short chain alkanols, increasing alcohol aggregation takes place with increasing the alkyl chain's length. We studied the aggregation behavior of various diols as a function of concentration and temperature, using the small-angle neutron scattering technique. Depending on the position of the OH groups and the length of the alkyl chain the structure of the aggregates is found to be very different. At lower concentrations, diols aggregate in a rather loose way, resembling statistical concentration fluctuations. At higher concentrations, the 1,2-diols organize themselves in lamellar structures, while this is not the case for 1,ω-diols. Triols with the three OH groups placed in one end of the molecule, can be supposed to form more micelle-like aggregates, due to their more pronounced amphifilic character. We measured solutions of 1,2,3-octanetriol and found that it forms rather compact aggregates. They can be modeled as interacting spherical objects, which can be tentatively identified as spherical micelles. The structures formed in diol solutions are not yet understood, more elaborated models should be searched.

Due to their specific properties in magnetic field, *ferrofluids* are widely used in different industrial, technical, as well as in biological and medical applications. A typical ferrofluid is a colloidal solution of magnetic particles (magnetite, cobalt, etc.) covered by either neutral or charged surfactant shell in a liquid carrier. The relationship between the characteristic

[#] Ph.D. student

size of the particles and interparticle interaction, especially under external magnetic field, determines the stability of the fluids in respect to sedimentation and coagulation. Small-angle neutron scattering (SANS) is an effective tool to study the structure of ferrofluids under a wide variety of experimental conditions. The most interesting effect observed in our study is the concentration dependence of the surfactant shell around the magnetic particles in the fluid magnetite/oleic-acid/benzene. The thickness decreases with the growth of the magnetic particle volume fraction, which reveals that the surfactant tails are more interlaced or pressed closer to the magnetite surface with the increase in the particle concentration. Ferrofluids on highly polar carriers (methylethylketone, water) are less stable. A specific aggregation depending on the fluid composition is observed in the initial samples even in the absence of magnetic field. A secondary aggregation in larger fractal complexes takes place in these fluids. The complexes are destroyed when the temperature increases. Magnetic field affects significantly the processes of the secondary aggregation. The observed time-changes in the scattering reflect the formation of elongated chain-like complexes. The interesting fact is that in some cases the growth of complexes continues in the same manner even, when the magnetic field is turned off.

Instrument development. — A new collimator system for the SANS instrument has been installed and put in routine operation. A special feature of this device is the multibeam focusing tube, providing important intensity gain.

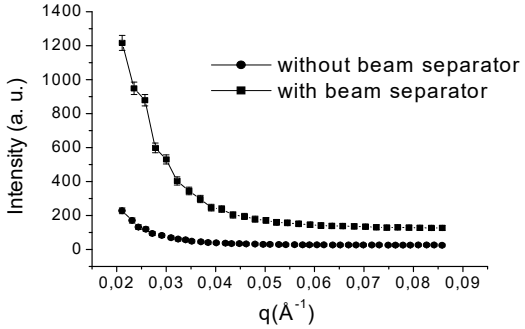

Figure 1. Tungsten sample measurements with 1 and 4 beams with the same time

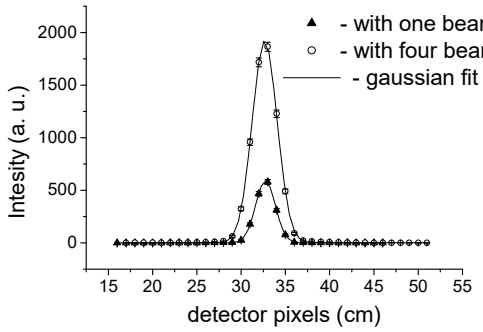

Figure 2. Gaussian fit of the direct beam profile with 1 and 4 beams at the wavelength of 4.91 Å

The aluminum separator and the inner surface of the collimator vacuum tube is coated with boron carbide. The cross-section of each beam is 8*8 mm^2 at the sample position. This setting can be used for measuring large, homogeneous samples, when the measurement does not need high spatial resolution. The beams are focused on the detector by appropriate diaphragms, the collimation length and the sample-detector distance is 4700 mm. In a real SANS experiment we have compared measurements performed on tungsten wire samples with and without beam separator (Fig.1). Using this beam multiplicator the measurement time can be reduced to a quarter (Fig.2) and can be achieved a factor of 4 (±15%) intensity gain.

Industrial application. — Welded joints have been scanned by a narrow neutron beam to get the SANS data for the base and welded metal. The cross sections have shown the presence of three fractions of particles having gyration radii: R_{g1} ~20 nm, R_{g2} ~9 nm и R_{g3} ≤ 1nm (point like defects). The amount of these defects was found in the base metal larger by a factor of 5 as compared to the welded metal. Assuming the existence of $Cr_{23}C_6$ precipitates, inducing the observed scattering, we estimated their content in the base metal, C_B=0.1% vol., corresponding to the amount of carbon C_{CB}=0.05 % wt. that is quite close to

the total concentration of carbon in the material (C_{Cmax}=0.07 % wt.). At the same time, in the welded metal the concentration of precipitates is very low, C_W =0.1 % vol. and only a small part (0.01%wt.) of carbon is precipitated. The observed size of large inhomogeneities agrees with the model of the clusters stacking into monolayers at the borders of grains and crystalline blocks. The figures below show the precipitate size distribution across the welded joint (Figure 3 and 4.

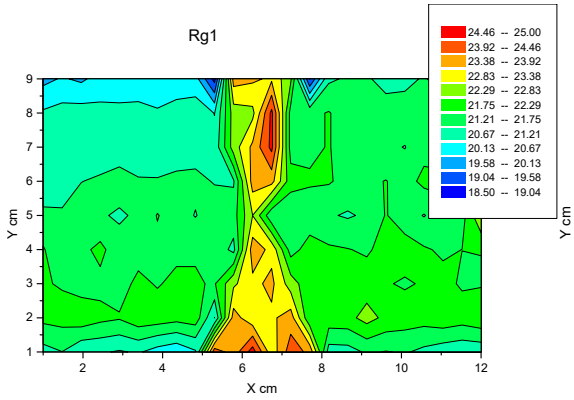

Figure 3. Particles distribution: R_{g1} ~20 nm

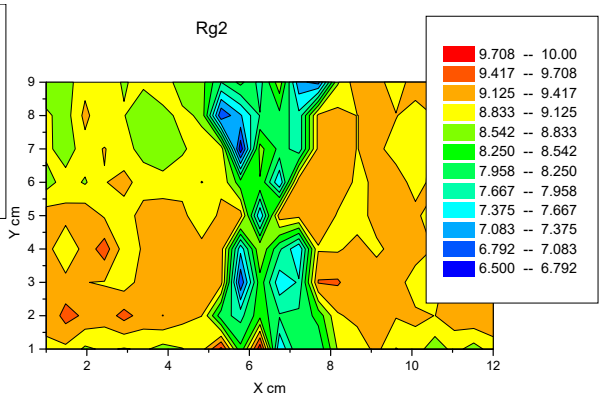

Figure 4. Particles distribution: R_{g2} ~9 nm

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Grants and international cooperations

EU HII3-CT-2003-505925 Acces to Research Infrastructure (BNC, L. Rosta, 2004-2007)
EU HII3-CT-2003-505925 JRA2 Detector Development project (L. Rosta, 2004-2007)
EU HII3-CT-2003-505925 JRA3 Focusing Neutron Optics project (J. Füzi, 2004-2007)
EU HII3-CT-2003-505925 JRA2 Polarised Neutron Techniques (Gy.Török, 2004-2007)
IAEA B5-HUN/8879 Condensed matter research (L.Cser, 2000-2004)
OMFB-00478/2004 Construction of Atomic Resolution Neutron Holography Instrument (L. Cser, 2004-2005)
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)
OTKA T 22486 Investigation of sintering processes (participant: E. Rétfalvi, 1999-2004)

HAS-RAS 10	(Hungarian-Russian bilateral) Cold neutron research (L.Rosta, 2002-04)
HAS-RAS 11	(Hungarian-Russian bilateral) Surface structures (L.Cser, 2002-04)
HAS-RAS 12	(Hungarian-Russian bilateral) Nanostructures (L.Cser, 2002-04)
HAS-RAS 25	(Hungarian-Russian bilateral) Water solvent structures by neutron and X-ray scattering (L. Almásy, 2002-04)
HAS-RAS 29	(Hungarian-Russian bilateral) Structure of biological macromolecular systems by neutron scattering (Gy. Török, 2002-04)
HAS-Dubna	JINR Dubna: SANS investigation of liquids (L. Rosta, 2002-04)
CNRS-HAS 17212	Study of clustering and cooperativity in aqueous solutions of uncharged species by neutron scattering and computer simulations. (L. Almásy 2004 - 2005)

Long term visitors

— M.V. Avdeev, senior scientist, Frank Laboratory for Neutron Physics, Dubna, Russia, January 1 – February 28 (host: L. Rosta)

— A.A.Khokhrykov, PhD student, T. Shevchenko University, Kiev, June 1- June 30 (host: L. Almásy)

Publications

Articles

J.1. Almásy L, Jancsó* G; Small-angle neutron scattering and Kirkwood-Buff integral study of aqueous solutions of pyridine; *J of Molecular Liquids;* **113**, 61-66*,* 2004

J.2. Avdeev* MV, Aksenov* VL, Kohlbrecher* J, Rosta L; SANS study of colloidal aggregates of silicon tetraethoxide in basic ethanol/water solutions; *Physica B;* **350**, e905-e908, 2004

J.3. Avdeev* MV, Khokhryakov* AA, Tropin* TV, Andrievsky* GV, Klochkov* VK, Derevyanchenko* LI, Rosta L, Garamus* VM, Priezzhev* VB, Korobov* MV, Aksenov* VL; Structural features of molecular-colloidal solutions of C_{60} fullerenes in water by small-angle neutron scattering; *Langmuir;* **20**, 4363-4368, 2004

J.4. Bica* D, Vékás* L, Avdeev* MV, Balasoiu* M, Marinică* O, Stoian* FD, Susan-Resiga* D, Török Gy, Rosta L; Magnitizable colloids on strongly polar carriers – preparation and manifold characteriziation; *Prog Colloids Polymer Sci;* **125**, 1-9, 2004

J.5. Cser L, Faragó* B, Krexner* G, I. Sharkov* I, Török Gy; Atomic resolution neutron holography (principles and realization); *Physica B;* **350**, 113- 119, 2004

J.6. Cser L, Török Gy, Krexner* G, Prem* M, I. Sharkov* I; Neutron holographic study of palladium hydride; *Applied Phys. Letter*s*;* **85**, 1149-1152, 2004

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J.10. Füzi J, Varga LK; Dipolar interactions in nanosized granular systems; *Physica B;* **343**, 320-324, 2004

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J.12. Füzi J, Kádár* Gy; A micromagnetic nanoparticle model of multiaxis anisotropy; *Physica B;* **343**, 293-297, 2004

J.13. Ionescu* C, Savii* C, Balasoiu* M, Popovici* M, Enache* C, Kuklin* A, Islamov* A, Kovalev* Y, Almásy L; Investigation of Silica - PVA xerogel microstructure evolution during thermal treatment by SANS experiment; *Acta Periodica Technologica;* **35**, 95-101, 2004

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K. NEUTRON SCATTERING

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

Barium-hexaferrites have continuously attracted a great scientific interest for decades, as their magnetic properties can be widely modified by substituting cations or their combinations into the structure. Our interest turned to the investigation of the rather complicated low temperature magnetic structure of Sc substituted Ba-hexaferrite. We have performed neutron diffraction structure study on $BaFe_{10.4}Sc_{1.6}O_{19}$ powder sample at 300 K and at 10 K. The crystal structure parameters could be refined in s.g. *$P6_3/mmc$*, and the distribution of Sc on the five cation sublattices (2a, $4f_2$,12k – octahedral, $4f_1$ – tetrahedral, 4e – bipyramidal) has been determined. The strong preference of Sc for the $4f_2$ site, secondly for the 2a site was established. The magnetic structure at 300 K could be well described by the ferrimagnetic Gorter-type order. At 10 K we observed extra magnetic reflections, indicating the change of the magnetic symmetry. In order to fit the pattern several magnetic models were tested, the best fit (Fig. 1.a) was obtained by a block-type, conical magnetic structure. Inside the blocks the magnetic moments are ordered ferrimagnetically, but their directions are declined from the hexagonal axis. The borders between the blocks are formed by the mirror planes of s.g. *$P6_3/mmc$* perpendicular to the hexagonal axis, and there is an antiphase coupling between the subsequent blocks. There is only one well-defined, isolated satellite reflection at 2Θ~9.6º (Fig. 1.b), which was indexed as (0 0 3+k), and for the k value approximately 0.24 was refined. For the cone angle ~40º was obtained, and the values of the sublattice moments were refined, as well. However, as the overlap of the mostly weak satellite reflections caused strong correlations, further measurements are needed to verify the quantitative results and the details of the magnetic ordering.

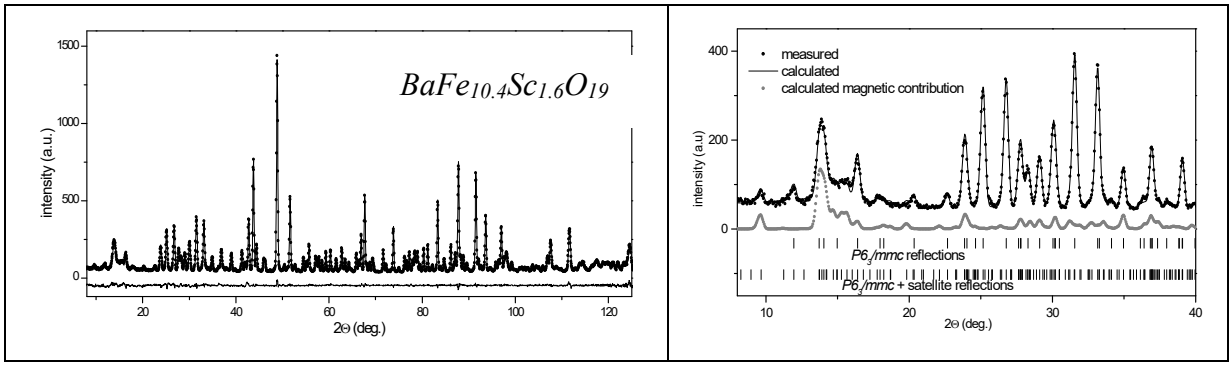

Fig. 1. a) Neutron diffraction pattern and Rietveld refinement of $BaFe_{10.4}Sc_{1.6}O_{19}$ (3T2/Saclay data λ=1.2251Å, 10K). b) Low angle part of the pattern together with the calculated magnetic contribution of the block-type, conical magnetic structure

Borosilicate glasses are of significant current interest as suitable materials for isolating host media for radioactive waste material storage. We have performed neutron diffraction structure study on a newly synthesized sodium borosilicate matrix glass system with general composition of *$65SiO_2*5B_2O_3*25Na_2O*5BaO$ (mole%)* doped with *CeO_2* and *ZrO_2*. Since *Pu* and *Ce* coordinations are rather similar in complex oxide environments, it can be expected that Pu coordination in a glass network is properly simulated by *Ce*. In order to increase both the hydrolytic and network stability of the matrix glass, *ZrO_2* was added. For data treatment to obtain the atomic pair correlation functions, both the traditional direct Fourier transformation technique and reverse Monte Carlo (RMC) simulation were applied.

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We have established that addition of CeO_2 to the host matrix did lead to formation of crystallites, embedded in the glassy network. With addition of ZrO_2 , however, the glass network could be stabilized. From RMC simulation of the neutron diffraction data we have obtained the partial atomic pair correlation functions for these multi-component glasses (Fig. 2). It was revealed that the short-range structure of the CeO_2 doped samples preserves the basic network configuration of the matrix glasses, making them suitable for radioactive waste material storage.

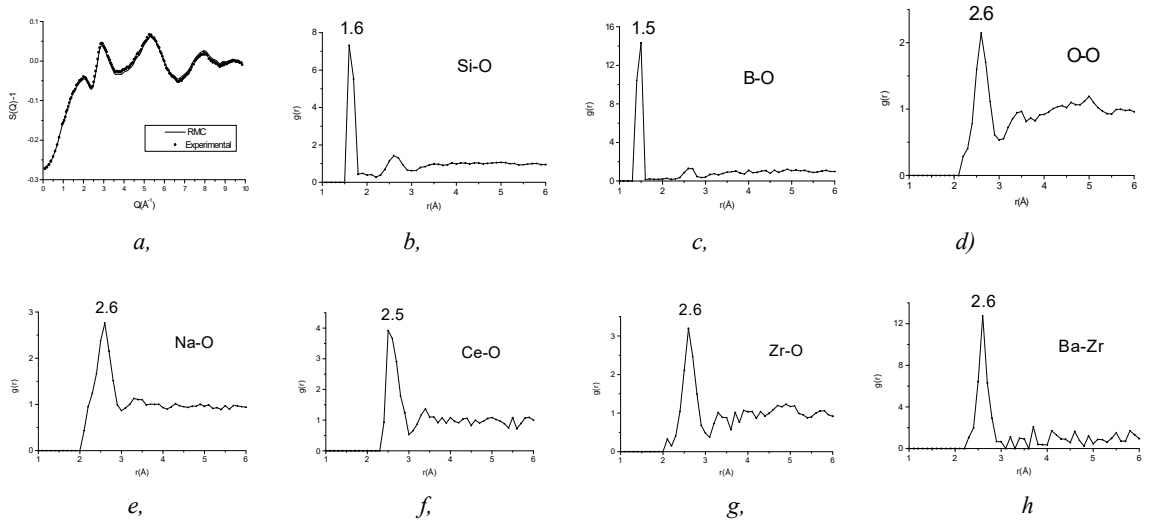

*Fig. 2. Glass 90%{60SiO_2*5B_2O_3*25Na_2O*5BaO*5ZrO_2}+10%CeO_2 : a/ Structure factor S(Q)-1, experimental (dots) and RMC simulation (solid line); b/Si-O, c/B-O, d /O-O, e/ Na-O, f/Ce-O, g/Zr-O, h/Ba-Zr partial pair correlation functions g(r), as obtained by RMC simulation.*

Liquids – Neutron diffraction data on *liquid carbon monoxide* (CO) and *nitric oxide* (NO), taken from the literature, have been analysed by means of the Reverse Monte Carlo method. From the resulting large particle configurations (containing 10000 atoms), partial pair correlation functions, molecular centre-molecular centre correlation functions and various orientational correlation functions could be calculated. It was found that in liquid CO, surprisingly well defined correlations exist between the orientations of molecular axes, particularly at higher densities. A transition from the dominance of 'T-shaped' constellations towards parallel ones was observed as a function of distance between molecular centres. Liquid NO was found to exhibit much shorter ranged correlations, mostly in the form of the 'T-shaped' constellations. The existence of $(NO)_2$ dimers – up to about 90 % - was found to be consistent with diffraction data. On the other hand, no significant proportion of 'cis-planar' type dimers is supported by our findings.

The structure of *aqueous hydrogen-chloride solutions* has been studied via RMC modelling, at several electrolyte concentrations. Partial pair correlation functions were calculated directly from the particle configurations. Based on the (water-)H-O partial it may be suggested that at very high electrolyte concentrations, HCl acts as a 'structure maker'. Concerning the hydration shell of the chloride ions, a straight O-H…D hydrogen bond angle was found at each concentration. As far as the coordination of the protons is concerned, it was demonstrated that the concentration of H_3O^+ species must be much less than it has been assumed previously.

Neutron diffraction data on *liquid carbon tetrachloride* served as a test case for studying the interplay between diffraction data and geometrical constraints in Reverse Monte Carlo simulations. Results indicate that diffraction data of limited momentum transfer can, indeed, be used to derive the structure of disordered materials with RMC modelling. In the interesting cases where the molecular structure has an important part in the definition of the intermediate range ordering, RMC constraints and diffraction data are competing/redundant. On one hand, this can be used to disentangle intermolecular from intramolecular features in the pair correlation functions. It can also help to detect systematic errors in diffraction data, or inconsistencies between different data sets. But, on the other hand, it must be kept in mind that the implementation of some RMC constraints (such as fixed neighbour constraints that can keep molecules together, coordination constraints or interatomic potentials) is partly arbitrary. Consequently, all RMC results must always be shown together with the set of constraints applied.

Internal stress - Quenched-in internal stresses have been determined in precipitated Cu grains in FeCu(5%) alloy as a function of the quenching temperature. The (111) reflection of Cu was considered, with attention paid to the line broadening. Significant differences are recognised in the developing stresses in the range of 850°C-200°C quenching temperature. The Cu grains are under tension in increasing degree with the quenching temperature. Between the extreme data a stress difference of 100 MPa can be determined while the total stress varies from 355 MPa to 280 MPa.

The line broadening also shows a peculiar behaviour in this temperature region. In contrast with the elastic stresses determined from the peak shift, these changes can be connected to plastic stresses or to the excess 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 (1.8 at% at 850°C) precipitates on the grain boundaries of the Fe grains. At lower temperature further Cu precipitates, but within the grains. These new and growing Cu grains with sizes up to ~1-2 μm contribute to the line broadening. These two processes, precipitation of Cu on the grain boundaries and within the grains, are responsible for the peculiarity of the broadening.

Radiography. — The use of non-destructive testing methods to qualify the state of rotor blades with respect of their expected flight hours – with the aim to extend their lifetime, without any risk of breakdown - is an important financial demand. In order to detect the possible defects in the composite structure of Mi-8 and Mi-24 type helicopter rotor blades used by the Hungarian Army, we have performed combined neutron- and X-ray radiography measurements at the Budapest Research Reactor. Several types of defects were detected, analysed and typified. Among the most frequent and important defects were observed cavities, holes and/or cracks in the sealing elements on the interface of the honeycomb structure and the section boarders. Inhomogeneities of the resin materials (resin-rich or starved areas) at the core-honeycomb surfaces proved to be an other important point. Defects were detected at the adhesive filling, and water percolation was visualized at the sealing interfaces of the honeycomb sections. Corrosion effects, and metal inclusions have been also detected.

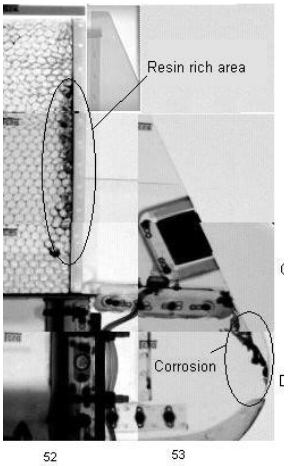

Fig.3. NR image of the rotor blade tail showing a resin rich area and spots of corrosion

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Long term visitors

— Guillaume Evrard, post-doctoral fellow, 01.01.2004. – 29.02.2004

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L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, S. Varró

Experimental research. — It is theoretically predicted that the carrier envelope phase ("absolute phase") of the short, few-cycle superintense laser pulses strongly affect the (multiphoton) interaction induced by such pulses. Recent experiments show that the dependence of the efficiency of high order multiphoton interactions on this "absolute phase" of the inducing few-cycle laser pulses is much weaker than theoretically predicted. We performed experiments to reveal the possible reasons of this discrepancy by producing three-photon photoemission of a polycystalline gold surface with few-cycle laser pulses of an intense Titanium:Sapphire laser. We registrated the relevant 3-rd order interferometric autocorrelation distribution of the photoemission. Unexpected "wings" appeared on the two sides of the autocorrelation curve (Fig.1) indicating a certain (~20 fsec long) life time lengthening suggesting ultrafast hot electron dynamics reducing the mentioned dependence of the efficiency of the high order multiphonon emission on the absolute phase.

Theoretical research. — On the basis of 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.

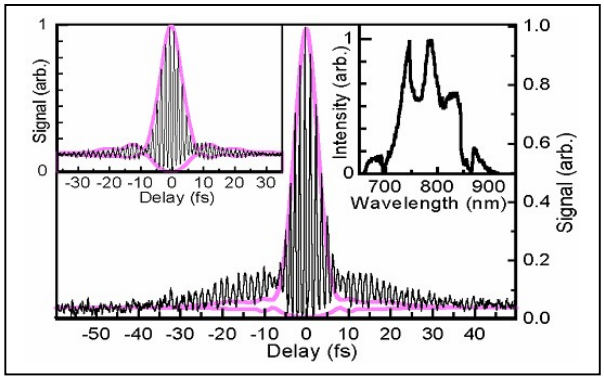

Figure 1. Measured third order autocorrelation curve of a 9.5-fs laser pulse using the polycrystalline gold surface. The thick contour line corresponds to the reconstructed envelope of the third order autocorrelation function of the pulse by fitting a polynomial spectral phase function. The left-hand-side inset shows a pulse diagnostic measurement carried out with a conventional second harmonic autocorrelator and the reconstructed envelope of the second order autocorrelation curve using the polynomial spectral phase function. The right-hand-side inset shows the spectrum of the pulse.

For some time now anomalous transparency induced by high intensity laser light interacting with solid foils has been found experimentally, and several theoretical models have been suggested to explain this phenomenon. In our theoretical study based mostly on classical elecrodynamics the increase of the transmittivity is the consequence of the more and more pronunced role of the frustrated total reflection in the plasma layer. We have given a detailed

analysis of the role of the electron temperature and the angle of incidence of the laser field. Our results nicely harmonize with the experimental findings.

We have derived explicit expressions for the Wigner funcions of wave functions in D dimensions corresponding to vanishing angular momentum that is of an s-wave. They are based either on the position representation or on the momentum representation of the s-wave. The corresponding Wigner functions depend on three variables: the absolute value of the D-dimensional position, momentum vectors and the angle between them. This is an unusual feature to compare with classical distributions. We illustrated this expression by explicitly calculating the Wigner function of a D-dimensional Gaussian, a ring-shaped wave function and that of a Wigner function of a free particle s-wave. Moreover, we have given the momentum distribution of the the generalized Neumann and Wigner type normalizable wave function in a completely repulsive potential, which have puzzled the physicist community for long (see von J. Neumann und E Wigner: Über merkwürdige diskrete Eigenwerte. *Physikalische Zeitschrift*, **XXX** , 465-467, 1929).

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Grants and international cooperations

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

DAAD Research Professor, Abteilung für Quantenphysik, Universität Ulm, Germany (S.Varró, 2 months, 2004)

Publications

Articles

L.1. Varró S; Scattering of a few-cycle laser pulse on a thin plasma layer : the effect of the carrier-envelope phase difference; *Laser Physics Letters*; **1**, 42-45, 2004

L.2. Varró S., Gál* KI, Földes* IB; Intensity dependent anomalous transmittivity of thin plasma layers; *Laser Physics Letters*; **1**, 42-45, 2004

L.3. Dombi* P, Krausz* F, Farkas Gy; Few-cycle-induced multiphoton photoelectron emission characteristics from a gold surface; *Appl Phys B*; accepted for publication

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Others

L.5. Dombi* P, Krausz* F, Farkas Gy; Ultrafast dynamics of multiphoton photoemission from gold and carrier-envelope phase sensitivy; In: *OSA 20th Anniversary Meeting, Advanced Solid State Photonics, 6-9 February 2005, Wien*; accepted for publication

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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. — Deep 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 is created in hollow-cathode discharges while the necessary metal atom density can be produced either by thermal evaporation or utilizing the cathode sputtering effect of the discharge. High-voltage hollow-cathode arrangements have been developed during the last ten-year 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. If we use lasers with this wavelength range the Raman and the flourescence spctrum can be separated. 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 have investigated the electric potential distribution and electron temperature in a steady state low-pressure helium discharge by means of emissive probe measurement. The breakdown characteristic (Paschen curve) of a hollow-cathode argon discharge has been studied with Monte Carlo simulation and experiments. In the field of strongly coupled plasmas we have studied the thermal conductivity of three-dimensional Yukawa plasmas in the liquid phase. For two-dimensional Yukawa systems we have investigated the structural (pair correlation function) and thermodynamic properties (correlation energy, compressibility) as well as the collective excitations through extensive molecular dynamics simulations. In cooperation with Portuguese and German groups we took part in studies of the comparison of different kinetic approaches for gas discharge simulations and possible applications of discharge based technologies in the field of surface treatment.

Electrolyte cathode atmospheric pressure glow discharge. — Using a tandem inductive coupled spectrometer (ICP) with a closed electrolyte cathode glow discharge (ELCAD) cell as nebulizer unit, it was possible to observe a well-defined element dependency of the cathode sputtering process on the electrolyte surface. Investigating the ICP signal ratio referred to the pneumatic nebulization, the ELCAD sputtering produces about three times higher mass transport for Al, Cr, Pb and Cd than for Mg and Cu. Ba, B, and Ca has even lower signal while Hg shows "super-sputtering effect" having 17 times higher signal with ELCAD than with pneumatic nebulization. Assuming that the positively charged particles are forced back to the cathode by the 10^7 Vm^{-1} field in the cathode dark space, these observations fairly fit to the model of the stepwise charge neutralization by hydrolysis taking place in the vapor phase, in the cathode dark space. This process, which is well known in the mass spectrometry, is determined by the character of the metal (M) – OH bond.

A vacuum system fitted multispectral imaging ellipsometer was developed in cooperation with the Research Institute for Technical Physics and Materials Sciences, HAS. In contrast to the usual ellipsometers, our outstanding technical parameters (2 seconds/5" diam. surface) make possible the real time control of production of microelectronic elements. The setup was successfully tested in Germany under industrial circumstances. Some practical modifications and preliminary experiments are in progress to increase further the speed and spatial resolution of measurements.

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Spectroscopy. — The role of *Stark effect* in the mode properties of hollow cathode (HC) lasers was analysed. It was found earlier, that while at the green He-Cd^+ HC laser Stark broadening gives a significant contribution to the homogeneous line-width resulting in single mode operation of this laser transition, at the blue one it does not. Recent studies on noble gas mixture HC lasers have given similar results: it was shown, that while at the He-Ar^+ 477 nm HC laser Stark-broadening has a significant role in single mode operation of this laser, at the He-Kr^+ 469 nm HC laser, though Stark broadening is also present, pressure broadening is enough large to explain this mode property.

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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)
OTKA T-042493	The role of ions of the basic electrolyte solution in the electrolytic cathode atmospheric pressure glow discharge (P. Mezei , 2003-2006)
OMFB IKTA-2000	Digital imaging spectroellypsometrical quality control arrangement (Z.GY. Horváth, 2001-2004)

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Articles

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M.2. Kalman* GJ, Hartmann P, Donkó Z, Rosenberg M*; Two dimensional Yukawa liquids: correlation and dynamics; *Phys Rev Lett;* **92**, 065001/1-4, 2004

M.3. Csillag L, Dimitrijević* MS: On the Stark broadening of the 537.8 nm and 441.6 nm Cd^+ lines excited in a hollow cathode laser discharge; *Appl Phys B;* **78,** 221-223, 2004

M.4. Pinhao* NR, Donkó Z, Loffhagen* D, Pinheiro* MJ, Richley* EA; Comparison of kinetic techniques for the analysis of electron swarm transport at low to moderate E/N values; *Plasma Sources Sci Technol;* **13**, 719-728, 2004

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M.6. Macko* P, Bánó G, Hlavenka* P, Plašil* R, Poterya* V, Pysanenko* A, Dryahina* K, Votava* O, Glosík* J; Decay of H_3^+ dominated low-temperature plasma; *Acta Physica Slovaca;* **54**, 263-271, 2004

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M.10. Hlavenka* P, Macko* P, Bánó G, Pysanenko* A, Plašil* R, Glosík* J; Cavity ring-down spectroscopy studies of plasmas; In: *Proceedings of 13th Annual Conference of Doctoral Students - WDS 2004, Charles University in Prague (Czech Republic) June 15 - 18, 2004*; Book of Proceedings, Ed: J. Šafránková, MATFYZPRESS, Prague, 2004, ISBN 80-86732-32-0; pp. 394 - 400, 2004

M.11. Kutasi K, Bibinov* N, von Keudell* A, Wiesemann* K; Wettabilities of plasma deposited polymer films; In: *Proc. of 17th Europhysics Conference on Atomic and Molecular Physics in Ionized Gases, 2-6 Sept. 2004, Constanta, Romania*; Eds.: V Ciupina, G Musa, R Vladoiu; pp. 273-274, 2004

M.12. Kutasi K; Molecular ions in helium glow discharges; In: *Proc. of 17th Europhysics Conference on Atomic and Molecular Physics in Ionized Gases, 2-6 Sept. 2004, Constanta, Romania*; Eds. V Ciupina, G Musa, R Vladoiu; pp. 23-24, 2004

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M.14. Donkó Z, Sadeghi* N, Baguer* N, Bogaerts* A; Measurement and modeling of spatial distribution of argon metastable atoms in a hollow cathode discharge; In: *Proc. of 17th Europhysics Conference on Atomic and Molecular Physics in Ionized Gases, 2-6 Sept. 2004, Constanta, Romania*; Eds.: V Ciupina, G Musa, R Vladoiu; pp. 161-162, 2004

N. METAL OPTICS

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

Surface plasmon oscillations and their statistical properties. — Near field microscopy of plasmons generated in different layer structures was performed by means of a scanning tunneling microscope (STM). For the first time the signal fluctuations are statistically evaluated. The direct plasmon signal shows a narrow Gaussian or Poisson-like distribution whereas the thermal signal of the plasmon oscillation is described by a Boltzmann type distribution as it is expected for a signal of thermal origin. The fact that narrow Poissonian structures are observed indicates that the generated plasmon radiation may have non-classic properties which unfortunately cannot be proven unambiguously with our setup.

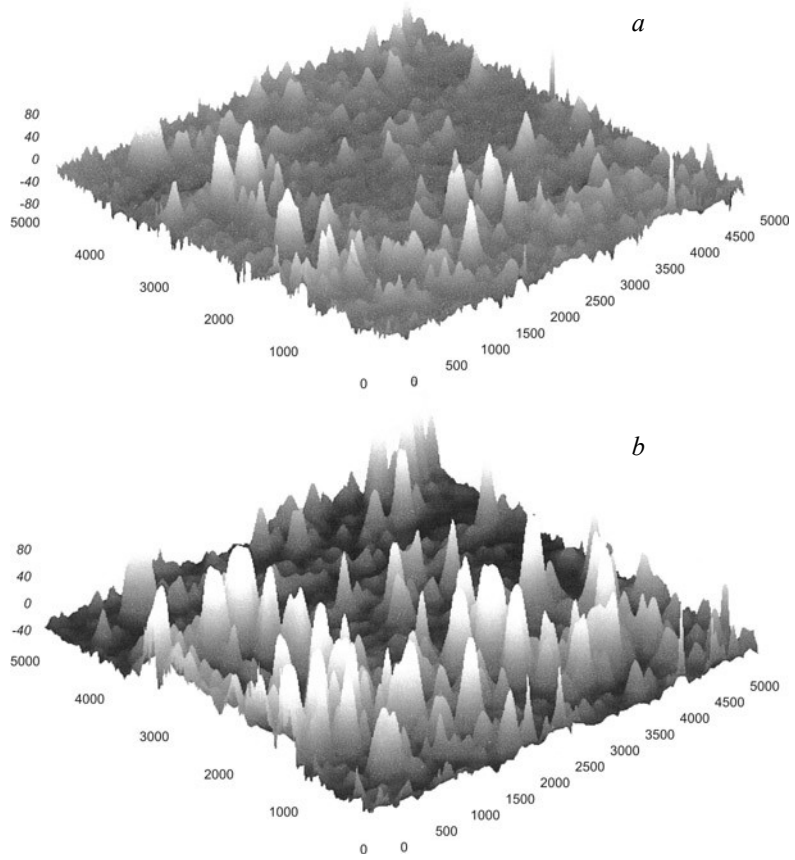

Figure 1. Surface plasmons created on a thin gold (mirror) layer, topography recorded in evanescent field (a) and a " thermal" map recorded simultaneously (b). The numbers in the X,Y,Z directions represent Å units.

For the excitation of surface plasmons (SPO) a 670 nm wavelength semiconductor laser has been used, chopped to get 50 μs long pulses with 1.8 kHz. repetition frequency. The response of the STM to the illumination has been detected in two time windows of 15 μs duration. The first time window has been placed at the onset of the laser pulse, when only the SPO signal was expected (with minor thermal influence) and the second one 40 μs after the laser has been switched off when only thermal (thermoelectric and thermal dilatation) effects can be seen. These two types of pictures are shown in Fig. 1a and 1b.

In the experiments vacuum evaporated gold and silver surfaces with thickness between 30 and 50 nm were used. Images have been taken for sample areas between 0.2 x 0. 2 μm^2 and 10 x 10 μm^2.

The research work was carried out in strong cooperation with the STM group of the Max-Planck-Institute für Quantumoptik, München.

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International cooperations

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.

Publications

Articles

N.1. Szentirmay Zs, Kroó N, Krieger* W; Preparation of silver tips for surface plasmon microscopy, *Central European J Phys*; accepted for publication

N.2. Kroó N, Szentirmay Zs, Walther* H; Sub-wavelength microscopy of surface plasmon oscillations and their statistical properties; *Surface Science;* accepted for publication

Article in Hungarian

N.3. Kroó N; Felületi plazmonok és közeli tér mikroszkópia; (Surface plasmons and near field microscopy, in Hungarian); Magyar Tudomány; **XLVIII**, 1096-1098, 2003

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. — The measuring head and electronic data acquisition and evaluation system of a new dual wavelength forward-backward scattering laser particle measuring instrument was developed for sizing, counting and for the estimation of the complex refractive index of aerosol particles in the sub-micron and micron size-range. In the instrument we used two different lasers (green and red), four detectors (forward and backward scattering for both wavelengths) and a special parabolic mirror.

Atmospheric pollution of the atmosphere. — In the frame of the National Research and Development Program (NDRP) a mobile laboratory for environmental monitoring of atmospheric aerosols and measurement of air contamination installed in a FIAT DUCATO microbus was equipped by a new aerosol sampler and a cascade impactor. Chemical analysis of the aerosols collected on the samplers makes possible the determination of their composition. During 3 measurement campaigns the peculiarities of the atmospheric contamination by aerosols were studied within the city of Budapest and its surrounding. The mass and number concentration, size distribution, composition and spatial distribution of aerosols measured in different locations during different seasons of the year were determined. Complete data bases, containing all collected results were created. The measured parameters were compared with the statistics of the asthmatic and bronchial disease diagnosed in the same locations during the same period. The correlation between the incidence of disease and aerosol contamination of the atmosphere was estimated. In the frame of this project airborne ambient aerosol measurements were carried out for the determination of scattered intensity amplitude and time delay distribution in different aerosol samples using a high time resolution detecting system. Calibration procedures and simulation algorithms were worked out. Research of a refined algorithm for the measurement of the direction of laser impulses in ambient air was continued.

Nanotechnology. — In the frame of the NRDP a high resolution interferometric surface testing system was developed based on a frequency stabilized He-Ne laser. An improved data evaluation and noise reduction system provides increasing the sensitivity of the interferometric phase detection Using this system a number of optical coatings, layers and special samples were studied with sub-nanometer resolution.

In the frame of this project high illumination small size light sources were searched for. Series of spectroscopic measurements were carried out for the evaluation of different frequency stabilisation schemes of semiconductor lasers. The previously developed photon correlation measurement apparatus was calibrated as to its size measurement sensitivity. The apparatus was proved to be sensible down to 100 *nano*meter particle size.

A quantum-optical measurement system for **testing of sensitive light detectors** using non-classical light was elaborated. The principle of a new pre-determined photon number light source was proposed. The laboratory experimental setup for such a new light source was constructed.

Amorphous carbon layers. — Ability of carbon atom to form different bonding hybridization is a crucial feature which governs macroscopic behavior of carbon containing matter. To map bonding characteristics of carbon atoms Raman scattering method is widely

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used. In spite of the numerous papers devoted to the Raman analysis of these materials, the interpretation of the D and G peaks contains many contradictions. One of the questions to be answered is the nature of the wide D peak, whether it is composite or not. Under special experimental conditions the sensitive surface enhanced Raman scattering (SERS) is able to detect the vibrations of small structural units and distinguish them by the selective enhancement. We have performed these experiments on hydrogenated amorphous carbon (a-C:H) and amorphous carbon (a-C) films. The results are shown in Fig. 1.

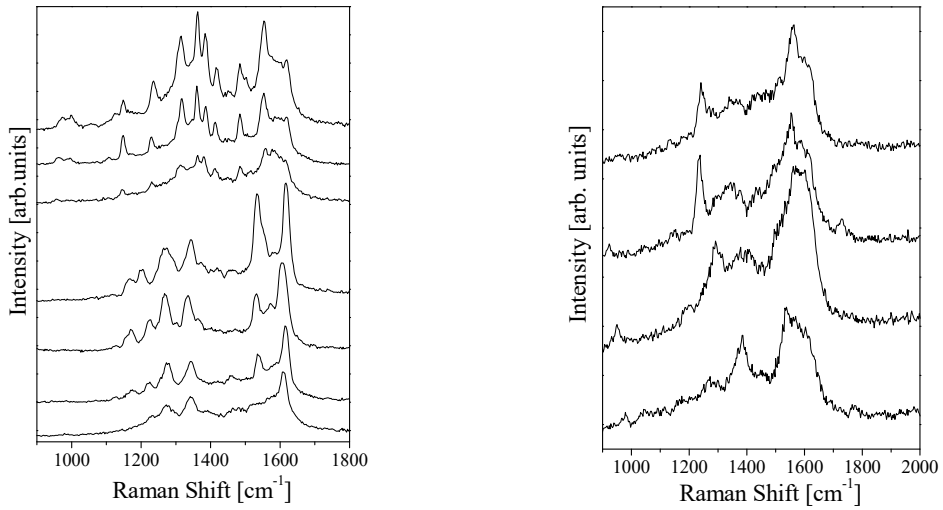

Figure 1. Surface enhanced Raman spectra of (a) a-C:H and (b) a-C films probed by 488 nm Ar ion laser line.

The SERS spectra display several new and important features: a) they demonstrate that the D and G peaks of a-C:H and a-C materials have composite character and built up of several bands; b) a considerable difference can be established between spectra of a-C:H and a-C, being more and narrow component peaks in a-C:H, in contrary to less and broad ones in a-C. These SERS results make questionable the existing interpretation of the D and G peaks as single ones as well as the characterization of amorphous carbon layers with the intensity ratios of the D and G peaks. Model calculations are proceeding in order to assign the component peaks.

In relation with biocompatible thin films development amorphous carbon layers were prepared on ultra-high molecular weight polyethylene (UHMWPE) surface by ion bombardment. An increase in the application potential of the UHMWPE may be achieved by producing a hard, wear resistant carbonaceous modified surface layer on it. In this study the surface of UHMWPE samples was treated by 1 keV N, H and He fast atom bombardment (FAB). The untreated and FAB-modified samples were studied by photoluminescence and optical absorption spectroscopy. The FAB-treatment caused a nearly complete disappearance of the characteristic luminescence bands of UHMWPE (3.70, 3.46 and 3.35 eV). The appearance of new bands at 2.5 and 2.7 eV suggests the formation of new recombination levels in the FAB-treated samples. From the remarkable decrease in integrated luminescence intensity the formation of a large number of non-radiative recombination states was concluded. Structural transformations caused by fast atoms resulted in the appearance of defect centers and corresponding localized deep levels in the gap, which act as radiative recombination states.

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Grants and international cooperations

OTKA T-043359 Preparation and complex characterization of carbon based nano-composites (M. Koós, 2003-2006)

NATO SfP-976913 Carbon based energy storage (M. Koós, I. Pócsik, 2000-2004)

Bilateral Hungarian-Ukrainian Cooperation, Contract No. UK-6/02 (M. Koós, I. Pócsik, 2003-2004)

NKFP-3A/042/04 National Research and Development Program– Development of new generation coronary stents on the base of clinical experiences, from haemocompatible materials coated by nanostructured coatings (Sub-coordinator: M. Koós, 2004-2006)

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

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

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

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

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

NKFP 3A/079/2004 National Research and Development Program — Nanotechnology (Sub-coordinator: A. Czitrovszky, 2004-2007)

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Articles

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O.19. Nagy A, Wu* J, Berland* KM; Photodynamics in fluorescence correlation spectroscopy; In: *Proceedings of Annual Meeting of the Biophysical Society, 14-18 February, 2004, Baltimore, USA*; pp. 436-439, 2004

P. FEMTOSECOND LASERS

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

Multilayers (1D nanostructures) in femtosecond and attosecond pulse laser systems. Continuing our research started in 1993, we investigated phase properties of Mo/Si multilayer filtering mirrors developed for single attosecond pulse generation experiments. For our studies in the 10 nm - 25 nm wavelength regime, which is typically used for single attosecond pulse generation, we used the following multilayer Mo/Si filter design: 30 bilayers of Mo and Si with spacing *d* of 9.1-9.5 nm with varying thickness ratios (Γ). In our calculation, Γ was defined as

$$\Gamma = \frac{d_{Abs}}{d_{Sp} + d_{Abs}}$$

in which equation d_{Abs} and d_{Sp} stand for the physical thickness values of absorbing Mo and the spacer Si layers, respectively. The computed spectral transmittance, reflectance and absorption of a multilayer Mo/Si filtering mirror with Γ = 0.17 is shown in Fig. 1a.

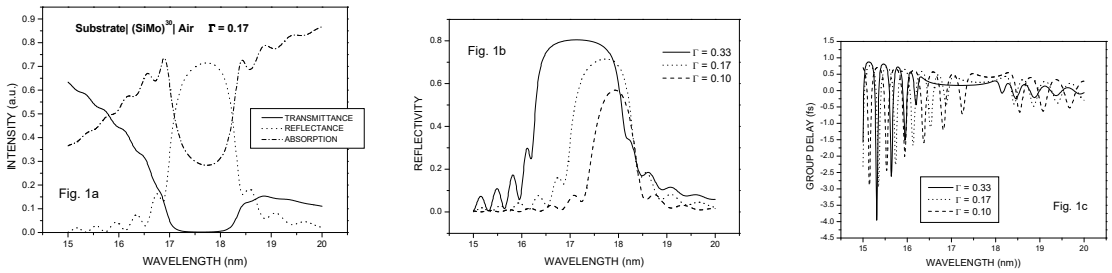

Fig. 1 Spectral transmittance, reflectance and absorption of a 30 bilayer Mo/Si filtering mirror with Γ value of 0.17 (Fig. 1 a), spectral reflectance (Fig. 1b) and group delay (Fig. 1c) of such mirrors with different Γ values of 0.1, 0.17 and 0.33

By varying the thickness ratio between the absorber layer d_{Abs} and the spacer layer d_{Sp}, while keeping a fixed bilayer thickness of about 10 nm, one can change the high reflectivity bandwidth of the multilayer mirror (see Fig. 1b). The corresponding (precisely) computed group delay versus wavelength functions are displayed in Fig. 1c. One can observe that the shape of group delay vs. wavelength functions follow that of the corresponding spectral absorption functions. Interestingly, the group delay variation Δτ over the reflectivity bandwidth of the mirrors does not depend on the Γ values, i.e., the cubic phase term reduces for higher bandwidth filtering mirrors.

Using the spectral reflectivity data $R(\lambda)$ shown in Fig. 1b and the spectral phase data $\varphi_{filter}(\lambda)$ used for calculating the group delay functions shown in Fig. 1c, we can compute the temporal shapes of single attosecond pulses being spectrally filtered by Mo/Si filtering mirrors of different Γ values. The results of calculations are shown in Fig. 2. The most dramatic change in the pulse shape can be observed in the case of the filtering mirror with Γ value of 0.1: the pulse duration increases from 286 as to 438 as (see Fig. 2a) due to the cubic phase and the pulse shape is strongly distorted (see Fig. 2b). This effect can be still recognized in the case of the Mo/Si multilayer mirror with Γ value of 0.17, when the pulse duration of the transform limited attosecond pulse is increased from 264 as to 314 as due to

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filter dispersion. In case of the highest Γ value (and highest bandwidth!), the effect of cubic phase can be neglected: this filter supports nearly transform limited pulse durations below 250 as.

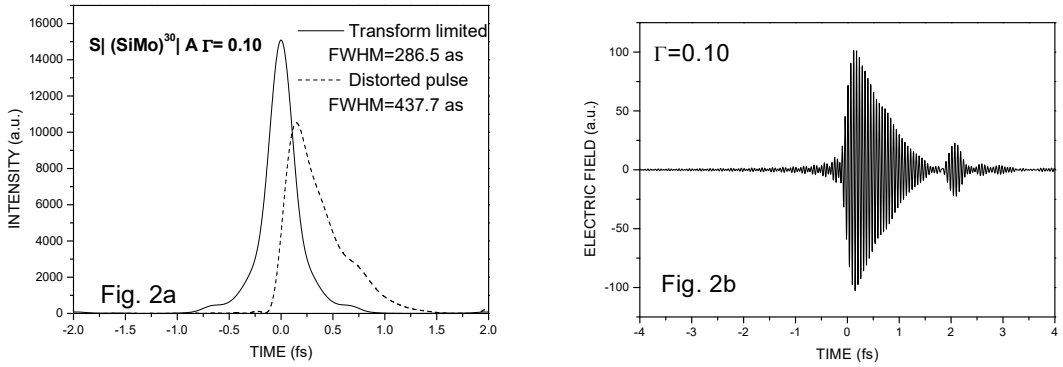

Fig. 2 The change of temporal pulse shape of single attosecond pulses being filtered by 30 bilayers of Mo/Si multilayer mirrors with Γ value of 0.1 (Fig. 2a). The computed electric field of the attosecond pulse being reflected on the filtering mirror with Γ values of 0.1 is shown in Fig. 2b.

Summarizing our results, we have shown that cubic phase distortion originating from narrow bandwidth ($\Delta E \approx 3$ eV) Mo/Si multilayer filtering mirrors results in longer time duration and multiple pulsing. Interestingly, this effect reduces for higher bandwidth filtering mirrors, i.e., for shorter attosecond pulses.

Pulse compression in 2D photonic crystal optical fibers. Continuing our research started in 2000, we investigated pulse propagation of femtosecond laser pulses in different photonic crystal fiber (PCF) structures. In our previous studies, we found that the compressed pulse duration was ultimately limited by the difference between the laser central wavelength (750 nm) and the zero dispersion wavelength (767 nm) of our PCF sample. By application of recently developed commercial PCF-s with red-shifted zero dispersion wavelengths, we demonstrated that it is possible to obtain sub-6 fs pulses at sub-nanojoule energy levels by optimization of input and output chirp parameters up to the third-order. Such input pulse energies with the required pulse durations can be easily obtained from low pump threshold, mode-locked Ti:sapphire laser oscillators pumped by a 532 nm pump laser with output power of as low as 1.3 W.

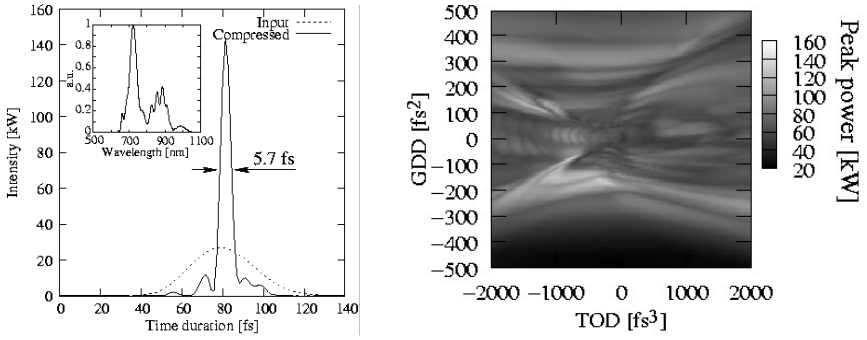

Fig. 2 Computer simulation results for pulse compression with a PCF: temporal input and compressed pulse shapes (left); output spectra (left, inset); optimization map (right).

One of the main results of our simulation is the following: if we apply 1 nJ, 12 fs input pulses with central wavelength of 760 nm, sub-6 fs pulses can be generated using a PCF with a length of 6 mm and by proper dispersion compensation (see Fig. 2, left).

Accordingly, the input pulse energy had to be further reduced in order to get spectral shapes similar to that obtained with a 6 mm long PCF used in simulations. In this way, we obtained twofold compression starting from 24 fs pulses with GDD_{in}=400 fs^2 and TOD_{in} = -6000 fs^3. The measured and computed autocorrelation traces are shown in Fig. 3 (left) and corresponding spectra are plotted in Fig. 3 (right). In the inset, the retrieved temporal pulse shape is shown with FWHM pulse duration of 12 fs.

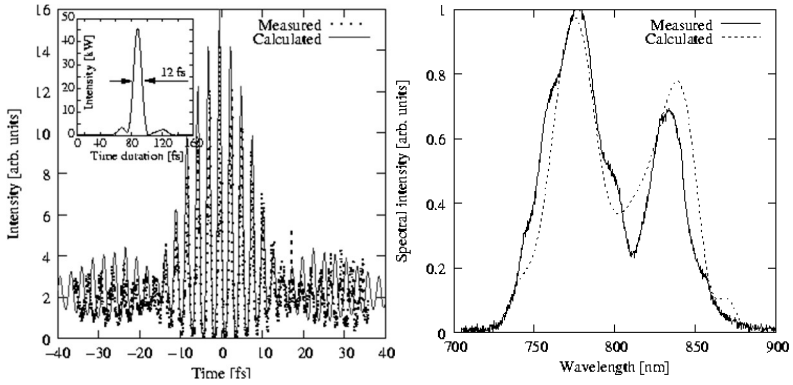

Fig. 3. Measured and computed autocorrelation traces (left) and the corresponding spectra (right). Input pulse parameters: 0.6 nJ, 24 fs. GDD_{in}= 400 fs^2 TOD_{in} = -6000 fs^3. Fiber length 22 mm. GDD_{out} - 320 fs^2 TOD_{out} -2000 fs^3.

The corresponding optimization map (see Fig. 2, right) shows the peak intensities of the compressed pulses as the function of pre-compression parameters (GDD_{in} and TOD_{in}), when an optimal compression is applied. The lightest areas show the highest peak powers that correspond to the shortest pulse durations. Because of practical issues, we could not fully provide the optimum experimental parameters we obtained from our simulations: our Ti:Sapphire laser operated at 797 nm, and provided 24 fs $sech^2$ pulses at a repetition rate of 76 MHz. A PCF piece with a length of 22 mm was the shortest that could be cut with our fiber cutter.

We can say that using commercially available photonic crystal fibers and cost effective, low pump threshold ($P_{pump} \approx 1.3$ W) Ti:sapphire lasers with sub-nanojoule pulse energies, it is feasible to generate compressed optical pulses in the sub-12-fs regime. Theory shows that by optimization of input and output chirp parameters, high quality, sub-6 fs pulses can be generated using a 6 mm long fiber piece. Further reduction of the compressed pulse duration at such energy levels seems to be feasible by application of new PCF-s with red-shifted zero-dispersion wavelengths and lower third-order dispersion values.

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Grants and international cooperations

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

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P.5. Fekete* J, Bányász Á, Szipőcs R, Katona* G, Lukács* A, Császár* B, Várallyay* Z, Sághy* A, Maák* P, Rózsa* B, Vizi* ES; Real time 3D nonlinear microscopy; In: *Proc. Advanced Solid State Photonics, February 6-9, 2005, Vienna, Austria;* accepted for publication

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See also R.5.

Q. OPTICAL THIN FILMS

K. Ferencz

Optical thin film structures consisting of nanoscale laminated layers. — We have continued our research concerning the development of optical thin film structures containing nanooptically thick layers for advanced applications in laser physics and information technology. We have refined our new electron-beam deposition technology for producing optical coatings containing nanooptically thick titania, silica, tantala, alumina, hafnia layers. Using needle-like optimization thin film design method, we have continued our research concerning the development of many kinds of ultrafast nanooptical coating systems – ultra-wide-band, low dispersion antireflection coatings, low dispersion beamsplitter coatings, ultrafast dichroic mirrors, wide-band output coupler mirrors, spectral shape filters for amplifiers, for example.

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

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 studied in cooperation with the Biophysics Institute at the Szeged Biological Research Centre, HAS (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 our Institute and Optilab Ltd.

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Contract

OPTILAB-SZFKI No. 1048/2004

Grants and international cooperations

NATO SfP 974262 Optoelectronic Devices Based on the Protein Bacteriorhodopsin (Coordinator: C.E. Wolf, Germany, 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, Szeged, 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, G. Dravecz[#], V. Horváth, Á. Péter, K. Polgár, O. Szakács, Zs. Szaller

Growth and study of nonlinear borate crystals. — BaB_2O_4 (barium metaborate) exists in two phases, and only the low temperature, non-centrosymmetric β-phase is adequate for non-linear optical applications. The α - β phase transition occurs by 170 ºC below the melting point. Therefore, the β-phase is generally grown from high temperature solution. Due to the high viscosity and related supercooling of the melt, it is possible to grow the β phase crystals directly from the supercooled melt. This technique, however, is extremely difficult and delicate, and it can only be realized at very steep axial and radial thermal gradients, and in a narrow melt temperature range. The preparation of the starting material by solid state synthesis, and the technological details of the Czochralski growth were elaborated. β-BaB_2O_4 single crystals were successfully grown by the direct Czochralski method. The best results were obtained with 140-160 ºC/cm inner and 550 ºC/cm outer axial gradients. The crystallization temperature was kept between 1030 and 1040 ºC. The largest crystals grown from a 50 cm^3 crucible were of 25 cm^3.

Single crystals of the self-frequency-doubling laser host, YAB ($YAl_3(BO_3)_4$), were grown by the top-seeded flux method, with Er and Dy dopants. The Er concentration varied from 0.05 to 12 mole%. The first high-resolution absorption spectra of Er in YAB are presented in the visible range and in the 9 - 300 K temperature range. The ground state of the Er^{3+} ions is $^4I_{15/2}$, and the energy levels and Stark components of 7 transitions to the $^4I_{9/2}$, $^4F_{9/2}$, $^4S_{3/2}$, $^2H_{11/2}$, $^4F_{7/2}$, $^4F_{5/2}$, and $^4F_{3/2}$ manifolds were analyzed and assigned. The number and shape of the sharp spectral lines at 9 K suggest that Er^{3+} ions uniformly occupy one specific lattice site (the trigonal prismatic yttrium positions) without detectable aggregation at higher dopant concentrations. The lattice parameters and atomic positions were determined by Rietveld refinement of the neutron diffraction patterns taken on powdered crystals. These investigations confirmed that the Er substitutes for Y even at high (12 mole%) Er content. Simultaneously, the Y/Er - O distances and the c lattice parameter changed by 0.001 Å.

Spectroscopic properties of the Dy^{3+}-doped $YAl_3(BO_3)_4$ crystal were determined from the vacuum-ultraviolet (VUV) to near-infrared spectral range. The spectra were interpreted in terms of the $4f^n$, $4f^{n-1}5d$ and charge transfer transitions. It was found that the VUV excitation was transferred to the optically active ions giving emission from the $^4F_{9/2}$ fluorescent level of Dy^{3+}. Unusual temperature variation of the Dy^{3+} fluorescence kinetics was observed, the $^4F_{9/2}$ lifetime increased with increasing temperature. The Dy-emission and its temperature dependence was explained by the assumption that the transition rates originating from individual crystal field levels of the $^4F_{9/2}$ emitting multiplet are significantly different.

Growth and study of stoichiometric and periodically polarized $LiNbO_3$ single crystals. — Growth condition of stoichiometric or near-stoichiometric $LiNbO_3$ from K_2O containing fluxes have been studied by investigating the phase equilibria in the K_2O-Li_2O-Nb_2O_5 ternary system. The limits of $LiNbO_3$ liquidus surface were determined by differential scanning calorimetry (DSC) and crystal growth experiments. In the region investigated, three ternary invariant reactions were found. A quasi-peritectoid reaction occurring at 966 °C: <$LiNbO_3$> + <$KNbO_3$> → <β–Li_3NbO_4> + <KLN solid solution>, a eutectic reaction

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at 997 °C: Liq. → <β–Li_3NbO_4> + <$LiNbO_3$> + <$KNbO_3$> and a quasi-peritectic reaction at about 1050-1055 °C: Liq. + <KLN solid solution> → <$LiNbO_3$> + <$KNbO_3$>. The liquidus-solidus tie lines of the $LiNbO_3$ phase field were established along the $LiNbO_3$-K_2O, $LiNbO_3$-E_t (eutectic point) and the $LiNbO_3$ - $KNbO_3$ vertical sections. The compositional path of the solidus lines was traced down to 1000 °C. From the constructed phase diagram both the compositional area and the yield of the growth of near stoichiometric $LiNbO_3$ single crystal were determined. Solidification with constant and near 50 mol% Li_2O composition was found only at the $LiNbO_3$-K_2O isopleth in the temperature range 1114 - 1000 °C. The conditions of the formation of stoichiometric and near-stoichiometric $LiNbO_3$ single crystals from high temperature solution are optimal in this range.

As-grown periodically polarized $LiNbO_3$ single crystals (PPLN) were prepared by the method of alternating polarizing electric field during the growth process. The effect of different technological parameters on the formation of periodic domain structure in Mg-doped congruent $LiNbO_3$ was investigated. It was shown that the quantity of the introduced dopants, the intensity of the poling current and the cooling circumstances of the crystals are decisive parameters in the preparation of as-grown PPLN. The size of the periods in the examined range of parameters was 25 - 30 micrometers (Fig. 1).

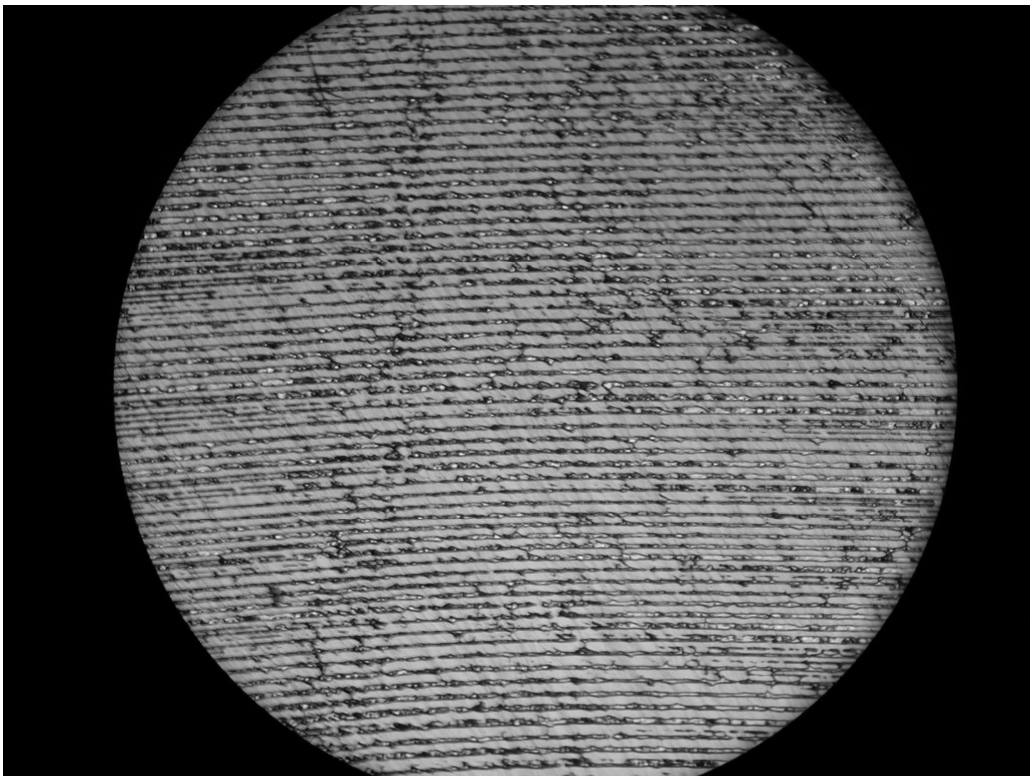

Fig.1.Etch pattern of a periodically polarized $LiNbO_3$ wafer.

Absorption and luminescence spectra of erbium doped $LiNbO_3$ single crystals have been measured and interpreted. From the optical absorption data the Judd-Ofelt intensity parameters for the f--f transitions of the Er^{3+} ions were determined, and the theoretical oscillator strength values of the Er-related optical transitions were calculated in the 350-850 nm range. From the luminescence excitation, emission and excited state lifetime data, an active mechanism for radiative energy transfer between the host crystal and the Er^{3+} has been identified.

Growth and study of bismuth tellurite crystal. — Bi_2TeO_5:Er single crystals were grown by Czochralski method. Optical absorption and emission spectra of Er^{3+} ions in Bi_2TeO_5

single crystals have been measured and analyzed. Besides the typical $^2H_{11/2} \rightarrow {}^4I_{15/2}$, $^4S_{3/2} \rightarrow {}^4I_{15/2}$, and $^4F_{9/2} \rightarrow {}^4I_{15/2}$, emission under excitation to higher energy manifolds than the actual emission, the $^4S_{3/2} \rightarrow {}^4I_{13/2}$ luminescence, that terminated to an excited state, was also detected. The energy levels of the $^4F_{3/2}$, and $^2H_{9/2}$ manifolds could be identified from the luminescence excitation spectra. These transitions were hidden by the absorption edge of the host crystal in the absorption spectra. The characteristic fine structure of the $^4S_{3/2} \rightarrow {}^4I_{15/2}$ luminescence provided good basis to determine the entire ground state Stark splitting. Judd-Ofelt (JO) calculation was performed to estimate the radiative transition probabilities, branching ratios and radiative lifetime of the transitions of Er^{3+} ions in Bi_2TeO_5 using the room temperature absorption data. The calculated Ω_t JO parameters were consistent with the preferential Er^{3+} substitution for Bi^{3+} sites in the Bi_2TeO_5 crystal structure. Comparing the JO parameters with those of other Er^{3+} doped laser crystals, it was concluded that the $^4F_{9/2}$, $^4I_{15/2}$, $^4S_{3/2}$, $^2H_{11/2} \rightarrow {}^4I_{15/2}$ and the $^4S_{3/2} \rightarrow {}^4I_{13/2}$ emissions may allow laser effect.

A new reaction pathway was identified in the solid state chemical reaction between powdered Bi_2O_3 and TeO_2 by DSC and electron microprobe analyses. In this system Bi_2O_3 was the stationary while TeO_2 the moving phase. Parallel to the grain boundary diffusion, TeO_2 layer was formed on Bi_2O_3 particles by the evaporation of TeO_2 above 450 ºC. The reaction sequence was independent from the starting composition, always the TeO_2 rich phases formed first. Bi_2TeO_5 could not be detected until the TeO_2 was fully reacted. The metastable phases identified during the reaction were β-$Bi_2Te_4O_{11}$ and $Bi_2Te_7O_{17}$.

Application of analytical methods for optical crystals and other media. — Solid sampling GFAAS (gas phase atomic absorption spectroscopic) method was elaborated for determination of Cr content in $LiNbO_3$ crystals. This method is based on dispensing a few mg powdered samples into a graphite platform, and then weighing and inserting the samples into the graphite furnace atomizer of the AAS system. The calibration was made by standard aqueous solutions of Cr, applying the three-point-estimation standard addition method.

The graphite furnace atomic absorption spectrometry was applied for the determination of Se in natural and Se-enriched cereals and bakery products. A robust and sensitive flow injection hydride generation method was developed. After digesting the samples, the Se content was separated in form of H_2Se. The decomposition of H_2Se, the trapping and atomizing the Se were optimized in a transversally heated graphite atomizer.

Complex sample collecting and analytical technique were developed and applied to determine the size, chemical composition and abundance of individual particles responsible for the deterioration processes on displayed artworks. The investigations in the church of Rocca Pietore (Italy) have shown that the use of hot-air “blow-in” heating system represented a major risk for plastered walls through the re-suspension of the particulate pollution, and the generation of NO_2 gas.

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Grants and international cooperations

OTKA T-034176 Preparation and investigation of nonlinear optical crystals and crystal structures (K. Polgár, 2001-2004)
OTKA T-046481 Growth and spectroscopic investigation of self-frequency-doubling laser crystals (I. Földvári, 2004-2007)
OTKA T-046667 Materials and systems for high density data recording (participant: I. Földvári, 2004-2006)
OTKA T038017 Development of laser ablation and electrothermal sample introduction methods for the atom spectrochemical study of element distributions (participant: L. Bencs, 2002-2005)
OTKA T-032339 Optimization of the parameters of the acousto-optic tunable filters (participant: Á. Péter, 2000-2004)
Hungarian Ministry of Education Research Program, OM-DDKKK 00004/2000 (participant: Á. Péter, 2001-2004)
Hungarian Széchenyi National Scientific Research Fund (NSRF) OM Grant No. 224/2001 Nanotechnology: Nonlinear crystals (contributor: Á. Péter, 2001-2004)
COST Action P8 (multinational EC program) Materials and systems for optical data storage and processing (I. Földvári, 2002-2005)
EC-project No. EVK4-CT-2001-00067. Friendly heating (contributor: L. Bencs)
HAS- Russian Academy Project 18. Investigation of crystal defects in broad forbidden band crystals (contributor: K. Polgár, 2002-2004)
HAS- Russian Academy Project 19. Solid state lasers (contributor: K. Polgár, 2002-2004)
HAS-Polish Academy Project 13. Investigation of structural defects in laser crystals. (contributor: E. Beregi, 2002-2004)
HAS - CNR (Hungarian-Italian bilateral) Growth and spectroscopic investigation of self-frequency-doubling laser crystals (I. Földvári, 2004-2006)
Hungarian - Italian Intergovernmental S & T Cooperation Programme. Growth and FTIR spectroscopy of optical crystals (conributor: I. Földvári, 2004-2007)
NATO Scientific Fellowship Program 4016/NATO/03. (L. Bencs, 2003-2004)

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R.10. Péter Á, Polgár K, Ferriol* M, Pöppl* L, Földvári I, Cochez* M, Szaller Zs; Ternary system Li_2O-K_2O-Nb_2O_5 Part II.: Growth of stoichiometric lithium niobate; *J Alloy & Comp*; accepted for publication

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R.13. Álvarez E*, Sosa R*, Földvári I, Polgár K, Péter Á, Munoz* AF; Judd-Ofelt analysis and energy transfer mechanism in $LiNbO_3$: Er^{3+} single crystals; *Phys Stat Sol (c)*; accepted for publication

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Conference proceeding

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Conference proceeding in Hungarian

R.16. Ajtony* Zs, Szoboszlai* N, Bella* Zs, Bolla* Sz, Bencs L; Gabonák és sütőipari termékek Se tartalmának vizsgálata FI-HG-GFAAS módszerrel (Study on the

selenium content of cereals and bakery products by FI-HG-GFAAS method, in Hungarian); In: *Proc. of the 46th Hungarian Conference on Spectrochemistry, Szeged, 2003*; pp. 30-35, 2003

Others

R.17. Hebling* J, Kuhl* J, Péter Á, Polgár K; Temperature dependence of the absorption and refraction of Mg-doped congruent and stoichiometric $LiNbO_3$ in the THz range; *CLEO/IQEC and PhAST Techn,16.-21. May 2004. San Francisco, California, USA*; Digest on CDROM 2004, CTh T33, ISBN: 1-55752-770-9

R.18. Bencs L; Book review: "Atomic Spectroscopy in Elemental Analysis"; In: *X-Ray Spectrometry;* (ed: M. Cullen); 2004, accepted for publication

See also K.9., S.3., S.8., S.14., S.15., S.16., S.20. 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

Microscopic quality of as-grown YAB crystals. — In undoped and doped $YAl_3(BO_3)_4$ single crystals grown from ($K_2Mo_3O_{10}$ + B_2O_3) flux the typical macroscopic as-grown imperfection is the random occurrence of opaque regions caused by foreign phase precipitations of microscopic scales. It was established by evaluating transmission electron diffraction patterns that the main foreign phase precipitations reducing the quality of YAB crystals are most probably: $KMoO_4$, $Y_5Mo_2O_{12}$ and $Y_4Al_2O_9$. The effective distribution coefficients **k** for the matrix and numerous dopant elements of YAB crystals were obtained using atomic absorption spectroscopy and electron beam microanalysis. Our **k**-values depend on the presence of (co)dopants and agree acceptably with literature data.

Point defects in oxide crystals. — $ZnWO_4$, $ZnWO_4$:Fe and $ZnWO_4$:Mo crystals were investigated by methods of time-resolved spectroscopy in the temperature range of 4.2–300 K. It is shown that the Mo and Fe impurities significantly reduce the light yield of $ZnWO_4$. The main 2.5 eV emission of $ZnWO_4$ and the 1.77 eV emission band of $ZnWO_4$:Mo originate from the triplet excited state of the WO_6 and MoO_6 complex, respectively. In $ZnWO_4$:Fe,Mo the MoO_6 emission band is shifted to lower energies due to the perturbing influence of the iron impurity. No perturbing effect of Fe or Mo ions was observed for the main emission of $ZnWO_4$:Fe and $ZnWO_4$:Mo. The luminescence spectra and decay kinetics in $ZnWO_4$ and $CdWO_4$ under pulsed electron beam and pulsed nitrogen laser excitation have been investigated. The two-stage intrinsic luminescence decay observed under ionizing radiation excitation was due to two different self-trapped exciton configurations in these crystals. The role of Fe and Mo impurities for scintillation efficiency has been discussed.

Polarized optical absorption spectra in $KHo(WO_4)_2$ single crystals were measured between 1.1 K and 300 K in the spectral range from 6,000 cm^{-1} to 30,000 cm^{-1}. The optical absorption lines are attributed to the $4f^{10}$ electron configuration of Ho^{3+} ions consisting of several groups of narrow lines similarly to the case of free Ho^{3+} ions, but due to the monoclinic symmetry of the crystal field these terms completely split into singlets. The energy positions and halfwidths of the observed 159 holmium sublevels were tabulated and their polarizations determined. The excitation spectrum is related to some lines in the absorption spectrum of potassium holmium double tungstates. Exciting the $^5I_4$ and $^5G_3$ states we studied the emission and discussed the Stark splitting of the ground level ($^5I_8$ for KHoW). A red shift of the luminescence was observed.

$LiNbO_3$ crystals doped with Mg in a wide composition range have been characterized by ultraviolet (UV) and infrared (IR) absorption spectroscopies. The results confirm that Mg eliminates Nb_{Li} antisites at the photorefractive threshold concentration. An approximate square root dependence of the OH^- band frequency versus Mg concentration was found for overthreshold samples independently from the Li/Nb ratio. The shift of the UV-edge to lower energies showed a linear dependence on Mg concentration superposed with a square root dependence on the concentration of Nb_{Li} antisites. Electron paramagnetic resonance (EPR) and optical absorption measurements on $LiNbO_3$ doped with Ti but containing also Mg to eliminate Nb_{Li} antisite trapping centres have shown that bipolarons may be trapped

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at Ti dopants. Bipolarons are formed if two electrons are trapped as self-compensating Ti_{Li}^{3+}–Ti_{Nb}^{3+} pairs on adjacent dopants on Li and Nb sites, or as Ti_{Li}^{3+}–Nb_{Nb}^{4+} units at neighbouring Ti_{Li} dopant and normal Nb_{Nb} sites. Experimentally they are manifested by opposite changes of the Ti_{Li}^{3+} and Ti_{Nb}^{3+} EPR signal amplitudes upon repeated partial oxidising–reducing or optical bleaching treatments.

The IR absorption spectra of the OH^- stretch-mode have been studied in a series of oxide crystals having optical applications. In $Sr_xBa_{1-x}Nb_2O_6$ and $Li_{1-5x}Ta_{1+x}O_3$ crystals the shape of the absorption band depends on x, allowing a simple non-destructive determination of the crystal composition. In $KHo(WO_4)_2$, $Bi_2(MoO_4)_3$ and $Pb_5(GeO_4)(VO_4)_2$ crystals the anharmonicity of the OH vibration measured on isotopically substituted samples was found to be in agreement with those in other oxides. The orientation of the OH^- dipoles in the crystals and the coupling of their vibration to lattice phonons have been determined.

Investigation of X-ray storage phosphors. — The new crystalline storage phosphor $BaCl_2$:Ce shows intense photo- and X-ray luminescence as well as efficient photostimulated luminescence which can be used for the readout of stored X-ray images. The emission is essentially related to a single active site of the Ce^{3+} activator which may be assumed to be charge-compensated by a monovalent alkali impurity as in the case of the A site in previously investigated $BaBr_2$:Ce. Much weaker luminescence due to intrinsic centres is also observed.

Thermal fixing and spatial distribution of wave mixing holograms in $LiNbO_3$. — The theory and a calculation method of four-wave mixing dynamic gratings were developed by introducing the complex response of the medium allowing the description of both local and non-local response and the regimes of stable, oscillating and chaotic solutions as well. All three regimes were reproduced by simulations. In the case of two-wave mixing general solutions were obtained for the grating amplitude profile and the output intensities, taking into consideration the absorption as well. By using these solutions, the topographic technique introduced by us previously became suitable for a quantitative characterization of photorefractive materials.

Design, recording and microscopic observation of optical gratings. — We developed a method for 'lapsed-time' determination of the temporal evolution of the profiles of photorefractive holographic gratings using both phase-contrast and interference microscopy. Amplitudes of higher-order harmonics as functions of bias exposure and recording fringe visibility were determined for phase holograms recorded in silver halide emulsions and processed using various schemes via phase-contrast microscopy and Fourier analysis. Dependence of refractive index changes caused by implantation of He ions in various glasses (IOG of Schott and a Tellurite glass) on the energy and dose of the implantation was determined. The results of the experiments can serve as a base for fabrication of various waveguide structures and gratings in these glasses.

History of science. — The history of crystal physics in Hungary was investigated from 1776 up to now. The results were presented at two international conferences and a Hungarian one. It came as a surprise to many, that although the word "crystallography" appeared only in 1802 in the English language (according to the "Encyclopaedia Britannica"), the "Crystallographia Hungarica" was already published in 1776.

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Grants and international cooperations

OTKA T 034262 Investigation and optimization of crystalline and glassy systems for data processing (G. Corradi, 2001-2005)
OTKA T 035044 Gyulai-Tarján school in crystal physics (E. Hartmann, 2001-2005)
OTKA T 037669 Geometrical, vibrational and electronic structure of borate crystals and their defects (A. Watterich, 2002-2005)
OTKA T 047265 Photo- and neutronrefractive materials and phenomena (L. Kovács, 2004-2007)
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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)
TéT Austrian-Hungarian Intergovernmental S & T Cooperation (A-8/2003): Photorefractive materials and phenomena for lights and neutrons (L. Kovács, 2004-2005)
TéT Italian-Hungarian Intergovernmental S & T Cooperation (I-46/03): Growth and FTIR spectroscopy of optical crystals (L. Kovács, 2004-2007)
TéT Italian-Hungarian Intergovernmental S & T Cooperation (I-15/03): Fabrication of active and passive integrated optical elements and devices by ion beam implantation (I. Bányász, 2004-2007)
HAS – Polish Academy of Sciences joint project: Structure of real crystals (A. Watterich, 2002-2004)
HAS – Polish Academy of Sciences joint project: Investigation of structural defects in laser crystals (L. Kovács, 2002-2004)
HAS – Estonian Academy of Sciences joint project: Electronic paramagnetic resonance and time-resolved luminescence spectroscopy of oxyanionic crystals (A. Watterich, 2004-2006)
HAS – CNR joint project: Growth and spectroscopic investigation of self-frequency-doubling laser crystals (I. Földvári, contributor L. Kovács, 2004-2006)
COST Action P8. Materials and Systems for Optical Data Storage and Processing (H.-J. Eichler (Berlin), Hungarian leader I. Földvári, contributor L. Kovács 2002-2005)

Long term visitors

— Irina Amin, University of Vienna, Austria, June 2004, 1 month (Host: L. Kovács)

— Mostafa Ellabban, University of Vienna, Austria, November 2004, 1 month (Host: L. Kovács)

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See also R.5., R.11.

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[#]

Cavity QED and laser cooling in resonators. — We considered an atom moving in a near resonant laser field with its dipole strongly coupled to a resonator field mode. As compared to the standard Doppler shift, we found a substantially different and counterintuitive linear velocity-dependence of the light scattering properties. The mechanical force of the laser field exhibits strong velocity-selectivity at a polariton resonance, which gives rise to an enhanced friction force and Doppler cooling even in the directions perpendicular to the resonator axis. This effect allows for sub-Doppler cooling of atoms even with a nondegenerate ground state.

We studied the axial motion of two atoms trapped at distant positions in the field of a driven standing wave high Q optical resonator. Even without any direct atom-atom interaction the atoms are coupled through their position dependent influence on the intracavity field. For sufficiently good trapping and low cavity losses the atomic motion becomes significantly correlated and the two particles oscillate in their wells preferentially with a 90º relative phase shift. The physical origin of the correlation can be traced back to a cavity mediated cross-friction, i.e. a friction force on one particle depending on the velocity of the second particle. We find joint trapping and cooling as well as fast thermalization of the two atoms. Choosing appropriate operating conditions allows for engineering these longe range correlations. In addition, this cross friction effect provides a basis for sympathetic cooling of distant trapped clouds.

Quantum information, entanglement and teleportation. — Entanglement is a genuine hallmark of quantum systems which has in recent years become one of the cornerstones of Quantum Information Technology (QIT). The relatively easy and efficient way to generate entangled photons has helped quantum optics to obtain a leading role in the study of the foundations of quantum physics and the implementation of QIT protocols. A possible way of representing quantum information in an optical system is the use of coherent-state superpositions as qubits. The advantage of this concept is that beam splitters can act as simple entangling gates. We introduced the adaptive Bloch sphere to analyze and visualize the effect of photon loss on coherent-state qubits. We then studied the robustness of the entangled coherent-state qubits created by a beam-splitter with respect to decoherence.

We have continued the research on the realization of quantum gates in various nano-structures, such as in SQUIDs and quantum dots. We have applied a previously developed quantum control scheme to chiral molecules to drive the molecule between its enantiomeric states. We have worked out the general theory of stimulated Raman adiabatic passage for degenerate systems. We have designed a new method for state preparation in a four state degenerate system, which combines the advantageous properties of optical pumping and adiabatic passage techniques.

Nuclear motion in molecules: dynamics and spectroscopy. — High-level ab initio electronic structure calculations, including extrapolations to the complete basis set limit as well as relativistic and diagonal Born-Oppenheimer corrections, resulted in a torsional potential of acetaldehyde in its electronic ground state. This benchmark-quality potential fully reflects the symmetry and internal rotation dynamics of this molecule in the energy range probed by spectroscopic experiments in the infrared and microwave regions. The

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torsional frequencies calculated from this potential and the ab initio torsional inverse effective mass function are within 2 wavenumbers of the available experimental values. Furthermore, the computed contortional parameter of the rho-axis system Hamiltonian is also in excellent agreement with that obtained form spectral analysis.

A simple variational procedure, termed DOPI for discrete variable representation-Hamiltonian in orthogonal coordinates-direct product basis-iterative diagonalization, is described and applied to compute low-lying vibrational band origins of triatomic molecules. Rotational constants characterizing these vibrational states have been also evaluated as expectation values using inertia tensor formulas in the Eckart and principal axis frames. The results show that it is the Eckart system that must be used in calculating the rotational constants.

Two methods are developed, when solving the related time-independent Schrödinger equation, to cope with the singular terms of the vibrational kinetic energy operator of a triatomic molecule given in orthogonal internal coordinates. The methods are applied to calculate vibrational energy levels above the barrier to linearity of the H_3^+ molecular ion, where singularities must be treated properly to obtain results of acceptable accuracy.

Quantum field theory in singular media. — Wave catastrophes are characterized by logarithmic phase singularities. Examples are light at the horizon of a black hole, sound in transsonic fluids, waves in accelerated frames, light in singular dielectrics and slow light close to a zero of the group velocity. We show that the wave amplitude grows with a half-integer power of the distance for monodirectional and symmetric wave catastrophes.

One can use transsonic Bose-Einstein condensates of alkali atoms to establish the laboratory analog of the event horizon and to measure the acoustic version of Hawking radiation. We have calculated the conditions for supersonic flow and the Hawking temperature for realistic condensates on waveguides where an external potential plays the role of a supersonic nozzle. The transition to supersonic speed occurs at the potential maximum and the Hawking temperature is entirely determined by the curvature of the potential.

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Grants and international cooperations

OTKA T034484	Application of nonclassical light in fundamental physical problems and in optical measurement methods (J. Janszky, 2001-2004)
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 T045955 Theoretical methods to describe vibrational-rotational motion of molecules (V. Szalay, 2004-2007)
TéT E/10-2001 (Hungarian-Spanish Bilateral Intergovernmental S&T Cooperation) Calculation of the rotational-torsional spectrum of molecules with asymmetric top and asymmetric frame, and analysis of overlapping spectral bands by filter diagonalization (V. Szalay, 2001-2004)
TéT CZ-5/03 (Hungarian-Czech Bilateral Intergovernmental S&T Cooperation) Representing and processing quantum information in quantum optical systems (T. Kiss, 2004-2005)
MERG-CT-2004-502887 (FP6 Marie Curie European Reintegration Grant of the European Commission) Collective dynamics of cold atoms in a cavity (P. Domokos, 2004-2005)
MERG-CT-2004-500783 (FP6 Marie Curie European Reintegration Grant of the European Commission) Hawking radiation in the laboratory: quantum field theory in singular media (T. Kiss, 2004-2005)

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See also: S.26.

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

The Institute hosts the *KFKI Condensed Matter Research Centre (KFKI-CMRC),* an organisation founded by four academic research institutes to co-ordinate the research activity in the field of condensed matter physics and application at the KFKI campus. The founders of the Centre are: the Research Institute for Solid State Physics and Optics, the Research Institute for Technical Physics and Materials Science, the Research Institute for Atomic Energy and the Research Institute for Nuclear and Particle Physics.

In 2000-2004, the KFKI-CMRC has successfully implemented a Centre of Excellence (CoE) project financed by the European Commission within the 5th Framework Program. The work conducted under the CoE umbrella was aimed at boosting international co-operation and improve links to other European centres. This was realised by actively organising workshops and conferences, reception of guest scientists for long or short time, visiting the co-operation partners and presenting the results in scientific journals and international conferences. The project started on the 1st of November 2000 and expired on the 28 of February 2004.

Altogether 12 *workshops/conferences* have been organised in the frame of the Centre of Excellence project, all with the participation of internationally acclaimed scientists and talented young researchers

The *long term visits* formed an essential part of the CoE project. Altogether 52 scientists have spent one month or more in the Centre. The average time was 4.6 months per visitor. The visitors arrived from 8 EU member states (majority from France and Germany) and from 5 former associated candidate countries (majority from Romania). More than half of the guest scientists was post doc or PhD student. A great number of visitors had spent a shorter time, typically 1 or 2 weeks at the Centre. The co-workers of the Centre realised 212 *missions* (conferences, workshops, discussions).

The intensive co-operation resulted in 109 *publications* acknowledging CoE (EC) support, all of them have been published in international journals (e.g. in the Physical Review B or E, the Physical Review Letters, and others). The co-authors represented 107 institutes in 23 countries. More than 30 papers have been published in conference proceedings or books.

The final report of project is available at the home page of the KFKI campus (http://www.kfki.hu/~cmrc/).

EDUCATION

Graduate and postgraduate courses, 2004

— Algebraic Bethe Ansatz and its application (F. Woynarovich, ELTE[2])
— Solid-state physics (J. Sólyom, ELTE)
— Renormalization methods for quantum systems (Ö. Legeza, ELTE)
— Advanced solid state physics I. (J. Sólyom, ELTE)
— Statistical physics (F. Iglói, SZTE[3])
— Applications of statistical physics (F. Iglói, SZTE)
— Disordered systems (F. Iglói, SZTE)
— Magnetism I. (P. Fazekas, BUTE[4])
— Magnetism II. (P. Fazekas, BUTE)
— Advanced solid state physics II. (I. Tüttő, ELTE)
— Electronic states in solids (J. Kollár, ELTE)
— Many body systems (P. Szépfalusy, ELTE)
— Solid state research I-II. (I. Vincze, ELTE)
— Amorphous and crystalline materials (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)
— NMR spectroscopy (K. Tompa, BUTE)
— Methods in materials science, neutron scattering (L. Rosta, BUTE)

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

— Neutron scattering in materals research (L. Rosta, ME[5])

— Neutron scattering (L. Cser, ELTE)

— Mathematical modeling in electrical engineering (J. Füzi, TUBV[6])

— Computer aided design (J. Füzi, TUBV)

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

— Applications of neutrons and synchrotron X-rays in condensed matter physics (L. Pusztai, L. Temleitner, BUTE)

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

— Optical information technologies (R. Szipőcs, BUTE)

— 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)

— The generalization of crystallographic groups (E. Hartmann, ELTE)

— Crystals and their non-linear optical properties (L. Kovács, PTE[7])

— Quantum mechanics I. (J. Janszky, PTE)

— Theoretical physics (P. Ádám, PTE)

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

— Solid state physics (P. Ádám, PTE)

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

— Statistical quantum optics (J. Janszky, ELTE)

— Nonlinear optics (P. Ádám, PTE)

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

Laboratory practice and seminars

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

— Atomic and molecular physics (K. Kádas, BUTE)

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

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

[5] ME = University of Miskolc

[6] TUBV = Transylvania University, Brasov

[7] PTE = University of Pécs

— 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 Gy. Tóth*, ELTE and BUTE)
— NMR (M. Bokor and P. Matus, BUTE)
— Electronics laboratory (M. Markó, BUTE)
— Laboratory practice in neutron scattering (A. Len, Gy. Török, BUTE)
— Computing in chemistry (L. Pusztai, ELTE)
— Laboratory practices in physics IV-V. (L. Temleitner, BUTE)
— Radiation protection laboratory practices (L. Temleitner, BUTE)
— Environmental protection laboratory practices: radiation aspects (L. Temleitner, BUTE)
— Medical application of lasers (Z. Gy. Horváth, E-D Medical Laser Center)
— Vector calculus 1 (P. Ádám, PTE)
— Vector calculus 2 (P. Ádám, PTE)
— Vector calculus 3 (Z. Kurucz, PTE)
— Vector calculus 4 (Z. Kurucz, PTE)
— Theoretical physics seminar (P. Ádám, PTE)

Diploma works

— M. Karsai (SZTE): Reaction-diffusion models in complex networks (Consultant: F. Iglói)
— A. Szállás (SZTE): Renormalization group study of aperiodic quantum spin chains (Consultant: F. Iglói)
— Á. Theisz (SZTE): Asymmetric simple exclusion process with particle creation and annihilation (Consultant: F. Iglói)
— G. Tóth (BUTE): Theoretical investigation of nucleation in the hard-sphere system. (Consultant: L. Gránásy)
— G. Katona (ELTE): Two-photon microscope for investigating components of neurons: dendrithic spikes and dendrites (Consultants: E.S. Vizi*, R. Szipőcs)
— G. Dravecz (ELTE): Top-seeded solution growth of potassium lithium niobate (KLN) crystals: Study of the phase relations in the ternary system of Li_2O-K_2O-Nb_2O_5 (Consultants: Á. Péter, K. Polgár)
— G. Czakó (ELTE): Exact quantum chemical calculation of molecular vibrations (Consultant: V. Szalay)

Ph. D. students

K. Radnóczi (BUTE): Effect of the relativistic spin-orbit interaction on orbital ordering phenomena in d-electron systems, in particular $BaVS_3$ (Supervisor: P. Fazekas)

F. Bagaméry (SZTE): Critical behavior on the presence of correlated disorder (Supervisor: F. Iglói)

L. Környei (SZTE): Percolative and dynamical properties of the random-field Ising model (Supervisor: F. Iglói)

P. Nagy (SZTE): Cooperation in complex networks (Supervisor: F. Iglói)

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

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)

G. Tóth (ELTE): Field theoretic description of far-from-equilibrium solidification morphologies (Supervisor: L. Gránásy)

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. 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)

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)

F. Szalai (ELTE): Strongly coupled plasmas: binary ionic mixtures (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, M. Koós)

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

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

A. Bahouka (Université de Metz): Comparative study of the physical properties of borate single crystals prepared by different methods (Hungarian supervisor: K. Polgár)

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)

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

Dissertations

L. Gránásy: Theoretical investigation of nucleation processes (D.Sc. Hungarian Academy of Sciences)

A. Kiss: Multipolar ordering in f-electron systems (Ph.D., BUTE, supervisor: P. Fazekas)

I. Pethes: Dissipation in $Bi_2Sr_2CaCu_2O_8$ high-T_c superconductors (Ph.D., BUTE, supervisor: G. Kriza)

P. Hartmann: Heavy-particle processes in low-pressure gas discharges (Ph.D., ELTE, supervisor: Z. Donkó)

Z. Jurek: Angstrom resolution imaging of atom clusters (Ph.D., BUTE, supervisor: G. Faigel)

H. Moussambi Membetsi: Growth of non-linear borates by the Czochralski method. First characterizations (Ph.D., Université de Metz, Hungarian supervisor: K. Polgár)

AWARDS

— I. Vincze, elected as Corresponding Member of the Hungarian Academy of Sciences

— M. Koniorczyk, Young Researcher Award of the Hungarian Academy of Sciences (2004)

— P. Domokos, Physics Award of the Hungarian Academy of Sciences

— Á. Bányász, EC Marie Curie Grant (2004-2005)

— P. Domokos, Talentum Prize

— T. Kiss, Gombás Pál Award (Roland Eötvös Physical Society, 2004)

— K. Kádas, titular associate professor of the Budapest University of Technology and Economics

— L.F. Kiss, SZFKI Annual Publication Award (2004)

— T. Pusztai, SZFKI Annual Publication Award (2004)

— P. Mezei and T. Cserfalvi*, SZFKI Annual Award for Applied Research (2004)

— M. Bokor, Bolyai Grant (2001-2004)

— L. Péter, Bolyai Grant (2004-2006)

— R. Szipőcs, Bolyai Grant (2004-2005)

— P. Domokos, Bolyai Grant (2003-2006)

— T. Kiss, Bolyai Grant (2003-2004)

— Z. Kis, Bolyai Grant (2003-2004)

CONFERENCES

— A two-days joint workshop "**On the topics of the scientific cooperation between the *Joint Institute for Nuclear Research*, Dubna, and the *Hungarian Academy of Sciences"*** was organised in collaboration with the KFKI-RMKI and the Roland Eötvös Physical Society on 6-7 September 2004 in Budapest, with participation of scientists from the Joint Institute for Nuclear Research (Dubna) and Hungary, aiming to present their most prominent results achieved during the last three years of the scientific cooperation. The three main topics presented and discussed in the workshop were: (1) Investigation of condensed matter by neutron scattering, (2) heavy ion implantation to solids and (3) theoretical nuclear and heavy ion physics. Besides the oral presentations, a booklet has been issued that contains 15 papers covering the whole field of the common scientific activity.

— The **European Aerosol Conference (EAC, Budapest, 6-10 September, 2004)** is a long-established meeting with high recognition joining the experts of different branches. Physicists, chemists, physicians, biologists, mathematicians and epidemiologists investigate the wide field of aerosols. This conference, with more than 600 participants, was organised this year in Budapest. The organiser was the Research Institute for Solid State Physics and Optics (Chairman of the Organising Committee was Dr. Aladár Czitrovszky) in co-operation with European Aerosol Assembly (EAA), Gesellschaft für Aerosol Forschung, Hungarian Academy of Sciences, National Council of Research and Technology, Hungarian Atomic Energy Authority, TSI Incorporated, Kálmán System Ltd. and Technoorg Linda Scientific Technical Development Ltd. During the Conference, 23 meetings of different Aerosol Associations and Societies were held.

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