ANNUAL REPORT

1999

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 1999

Edited by **L. Csillag, G. Konczos, B. Selmeci, E. Tóth-Kádár I. Tüttő,**

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Dear Reader,

It is my pleasure to hand over the Annual Report of the research activities of the Research Institute for Solid State Physics and Optics in 1999. This booklet is already the 6th Volume in a series of yearbooks of our Institute.

Our Institute was founded by the Hungarian Academy of Sciences in 1981 as part of the Central Research Institute for Physics. In 1992 we became an independent institute with the name : "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 reorganization process of the academic institutes and at the same time the name of the institute has been changed to "Research Institute for Solid State Physics and Optics".

The main profile of the Institute is to do basic research in the fields of theoretical and experimental solid state physics and materials science, including metal physics and liquid crystal research, theoretical and experimental optics, including laser physics and the interaction of light with matter. Our experimental research activity is connected to unique methodologies based on large and medium sized facilities like X-ray diffraction, NMR-, Mössbauer-, and optical spectroscopies and neutron scattering experiments at the KFKI Research Reactor.

Some of our research (R & D) activities are more closely related to applications, first of all in the fields of optical thin films, laser applications, crystal growing technologies and metallurgy.

Our research activity in the field of basic research is financed by the Hungarian Academy of Sciences and the National Research Fund (OTKA) through supporting individual projects. The participation of our research groups in international projects has become more and more significant in supporting our research. Our research groups have gained financial support from the National Committee for Technological Development, too.

In 1999 Hungary has joined the European Union 5th Framework Programme, and thus the international cooperation has become even more important for the scientific work of our research groups. We have living contacts with a great number of research institutions and universities. In more than half of our publications there are foreign co-authors indicating the significant role of these contacts. The different EU, ESF, COST, NATO and other international projects play a rapidly increasing role in our research activity. It is expected that the share of these resources in our budget will increase with the evolution of the integration process of our country. Our Institute has been taking part traditionally in gradual and to a larger extent in postgradual education. Details of this activity are also given in this Annual Report. We have published more than 180 papers in high quality international journals and conference

proceedings. This number of publications (per scientists) is similar to that in the previous years.

May 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 too, to make it easier to get in contact with them directly. For further information please visit our WEB-page.

Budapest, December 1, 1999

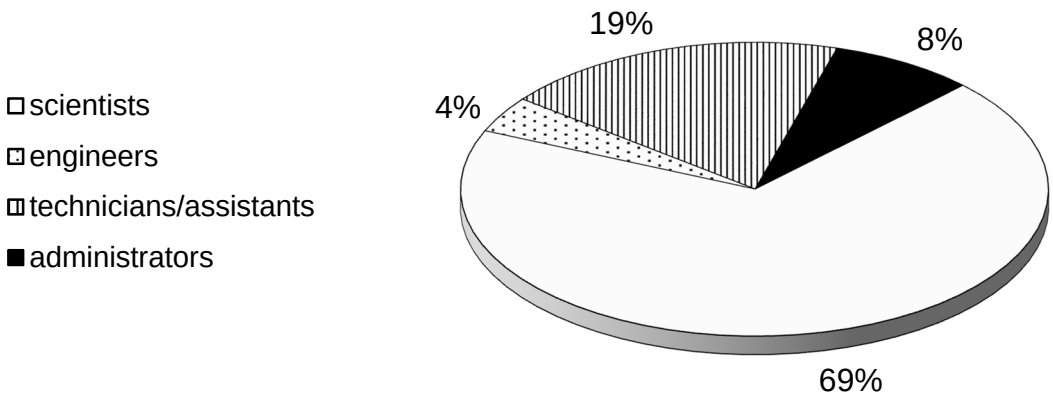
János Kollár

Director

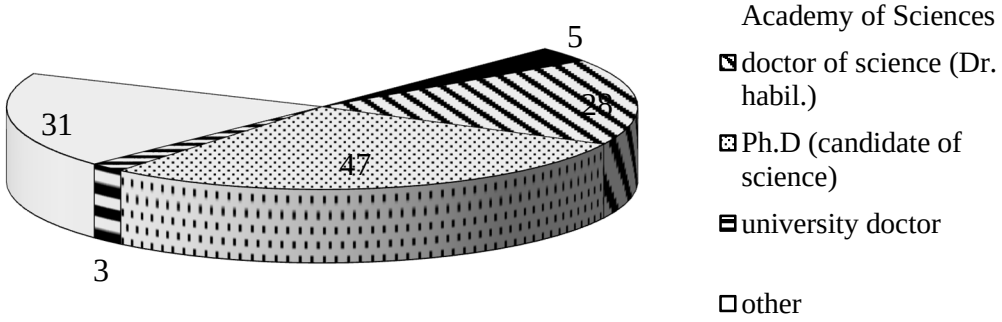
Key figures

Permanent staff of the Institute: 165 employees. Its distribution:

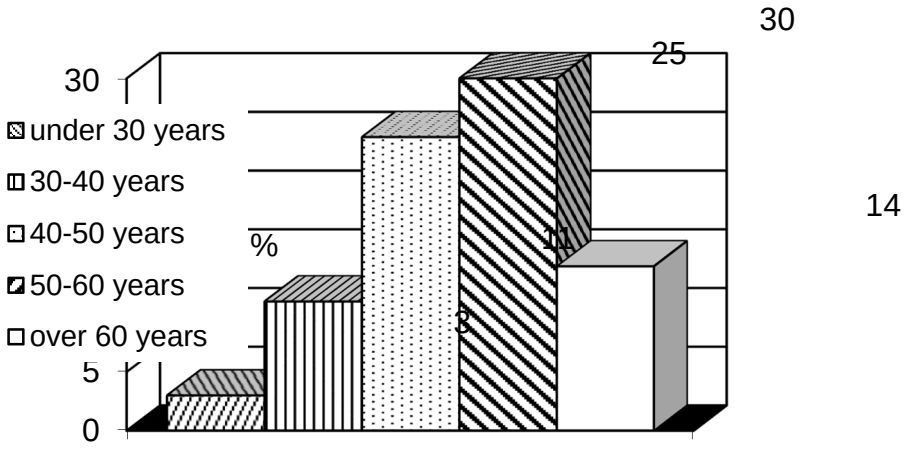
a) by professions:



b) by scientific titles/degrees:

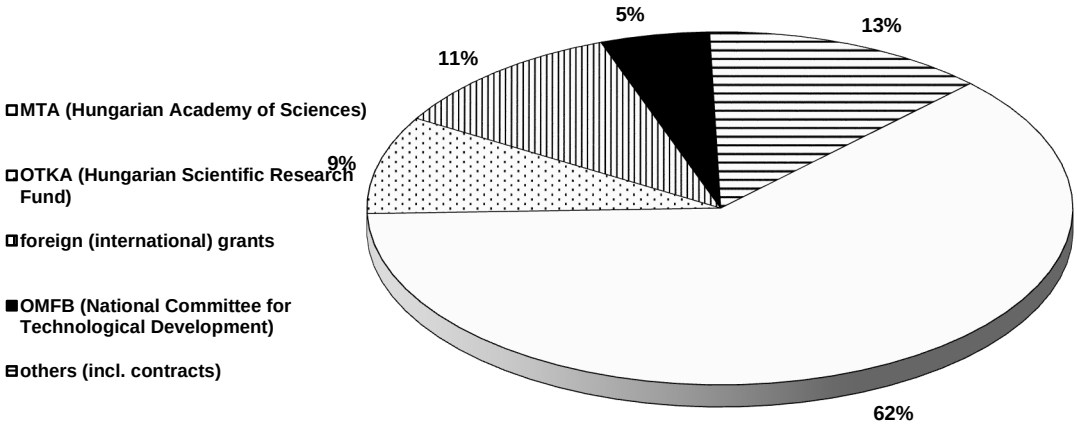


c) by ages:

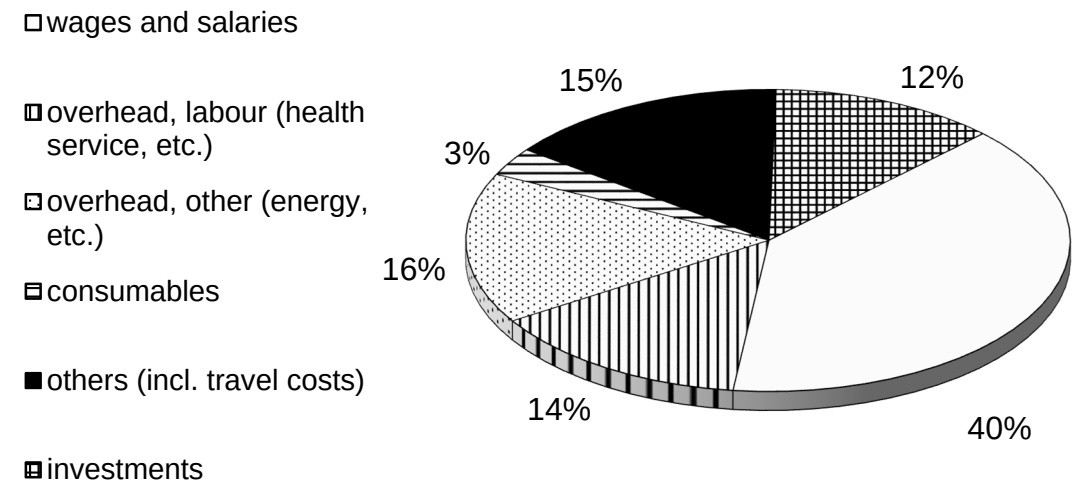


Financial management

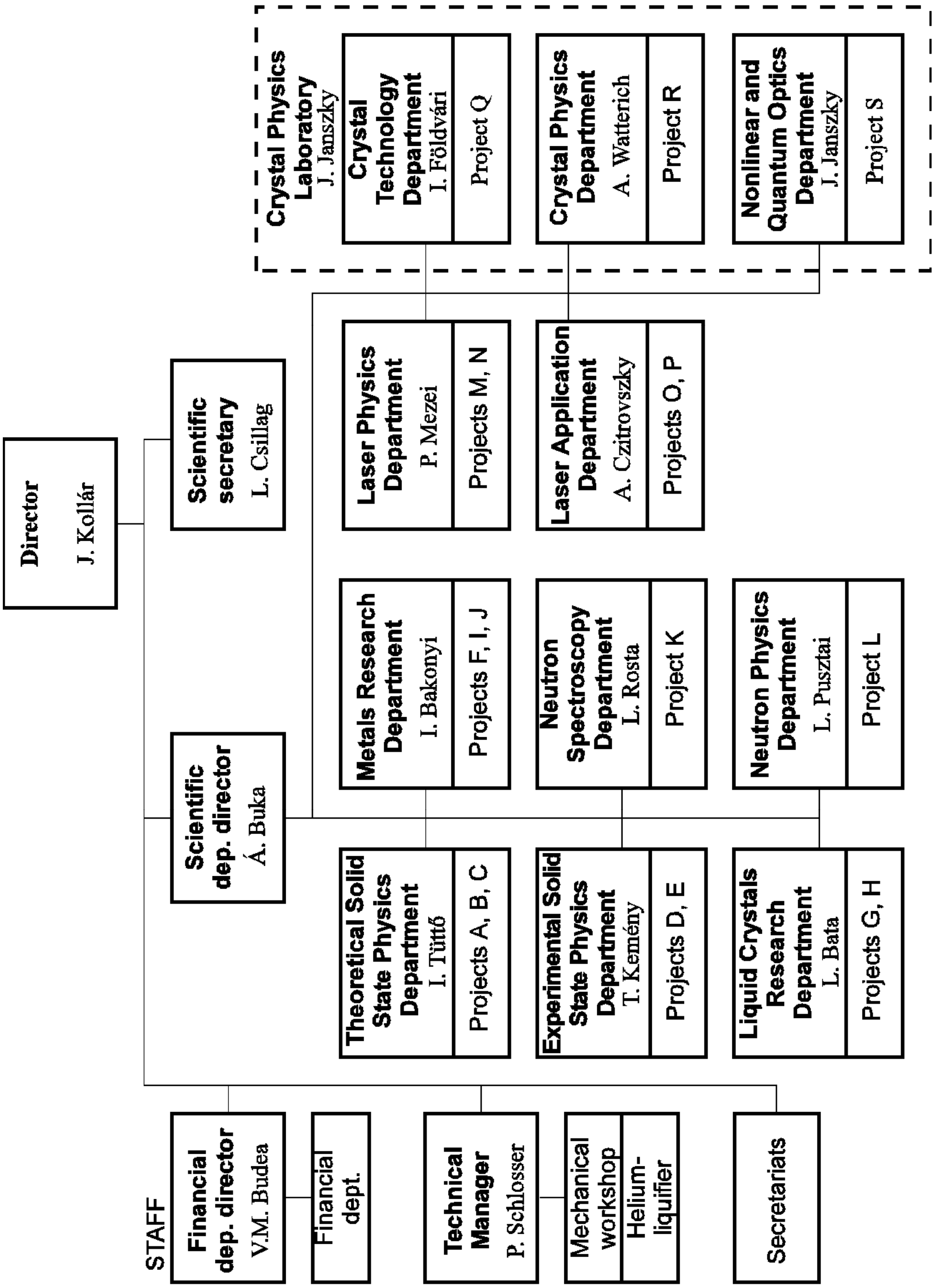
a) Sources of operation costs:



b) Distribution of expenditures:



Structure of the Research Institute for Solid State Physics and Optics



A. STRONGLY CORRELATED SYSTEMS

J. Sólyom, G. Fáth, Ö. Legeza, K. Penc, A. Rákos, K. Vladár, F. Woynarovich, A. Zawadowski[+]

Low dimensional magnetic models. — We have determined the phase diagram of S=1/2 anisotropic spin ladders. It is well established that isotropic antiferromagnetic spin ladders with odd number of legs remain gapless, while for even number of legs a Haldane gap is generated. We have shown that in latter case the two-leg ladder behaves differently from ladders with higher number of legs. In a two-leg ladder the inter-leg coupling is always relevant, generating a Haldane gap. For four-leg (six-leg, etc.) ladders this coupling is in general irrelevant, except for the special isotropic situation. The gap generation starts only at a finite value of the inter-leg coupling.

We have studied the low energy excitations of $CuGeO_3$ and have shown that to describe properly, one must include the effects of a transverse antiferromagnetic coupling, which was estimated to be $J_\perp$=0.15 J. Owing to this coupling the frustration in the chains is significantly lower than recent 1D estimates based on purely one-dimensional arguments, and we have found a strong modulation of the nearest neighbour coupling due to the static distortion, which is 5 times higher than that previously deduced from a 1D chain approach. By performing density-matrix renormalization group method (DMRG) calculations for 2 coupled chains we have analysed the effect of the transverse coupling on the ratio of singlet to triplet gaps. The ratio is very sensitive to the parameters and the universality reported in the strict one-dimensional case is lost.

The zero temperature phase diagram of a one-dimensional S=2 Heisenberg ferromagnet with single-ion cubic anisotropy was studied numerically using the DMRG. Evidence was found that although the model does not involve quadrupolar couplings, there is a purely quadrupolar phase for large values of the anisotropy. The phase transition between the magnetic and quadrupolar phases is continuous and it seems to be characterized by Ising critical exponents.

Using the XXX Heisenberg chain as a representative example we have studied the connection between the basic SU(2) symmetry of a model and the symmetry of the excitations. It was found, that the symmetry of the eigenstates can be explained supposing that the excitations obey SU(2) with a modified coproduct, or they obey a q-deformed SU(2) at q=–1. We started to examine the behaviour of the extremly low (O(1/N)) energy excitations of the XXX Heisenberg chain. We have found strong indications that the size of these excitations is of the order of the chain length.

Fermionic models. — Quasi-1D materials based on cuprate compounds, of which Sr_2CuO_3 is the best example, have become new candidates for ideal model systems which allow the study of basic physical concepts in one-dimension. Information on the electronic structure and the dynamics of the charge carriers is highly desirable, especially against the background of spin-charge separation expected in 1D. Beside the one-particle spectral function obtained by photoemission, the dielectric function is the most basic and important quantity reflecting the electronic structure of a solid. The dielectric response is accessible using electron energy-loss spectroscopy (EELS), offering the possibility to study the momentum dependence of the electronic excitations, i.e. the dynamical dielectric response.

[+] Permanent position: Technical University of Budapest

We have reported the first investigations of the dynamical dielectric response of Sr_2CuO_3 in collaboration with the experimentalists of the *Institut für Festkörper- und Werkstofforschung* in Dresden, and *Department of Superconductivity, The University of Tokyo*. We have carried out EELS measurements on single crystalline samples, which provides us with the energy and momentum dependent loss function Im $(-1/\varepsilon(\mathbf{q},\omega))$. While for small momentum transfer we see a broad continuum of interband plasmons above the gap, on the way to the zone boundary a sharp peak develops. We show that the data can be understood within an extended effective one-band Hubbard model and that both the spin-charge separation which occurs in 1D as well as excitonic effects are essential.

It is believed that some aspects of the electronic properties of the strongly correlated transition metal oxides, like manganites, can be revealed by considering the Kondo-lattice Hamiltonian with ferromagnetic exchange between the localized and itinerant electrons (Hund's rule). We have shown that the strong coupling limit of the Kondo lattice with infinite long range hoppings can be solved exactly using the underlying spl(2,1) dynamical supersymmetry. We learned that on this particular lattice (i) an extended Gutzwiller projection becomes exact, (ii) the ferromagnetic ground state is not favored. Finally, extending our result to more general lattices we arrived at an interesting conjecture that large density of states (e.g. Kagomé and pyrochlore lattices have flat bands in their one-particle density of states) is against ferromagnetism in the double exchange model.

Theory of dissipative motion of heavy particles. — We studied the Bloch wave diffusion of a heavy particle in fermionic environment. Path integral formulation and renormalization was derived by integrating on the fermionic degrees of freedom. The heavy particle localizes at strong dissipation, similarly to the case of two state system.

Other topics. — We studied cellular differentiation in a developing organism via a discrete bistable reaction-diffusion model. A system of undifferentiated cells was allowed to receive an inductive signal emanating from its environment. Depending on the form of the nonlinear reaction kinetics, this signal could trigger a series of bifurcations in the system. Differentiation started at the surface where the signal was received and either cells changed type up to a given distance or, under other conditions, the differentiation process propagated throughout the whole domain. When the signal was diminishing, hysteresis was observed.

We analysed the Ginzburg-Landau and Schrödinger equations with a nonuniform magnetic flux density, and showed that they admit a class of *internally-orthogonal*, - and in special cases - tracking solutions, where the gradient of the logarithm of the order parameter (wave function magnitude) is orthogonal to the gradient of the gauge invariant phase. For the macroscopic GL model virtually all solutions are in the internally-orthogonal class. In two dimensions, we found multi-fluxoid quantum vortex, dot and wall nucleation, and surface tracking solution. For the microscopic Schrödinger model we demonstrated that there exists a broad class of internally orthogonal, and closed form tracking solutions.

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Grants

OTKA[1] T017128. Theoretical study of dissipative motion of heavy particles (K. Vladár 1995-1999)
OTKA T022607. Completely integrable quantum chains (F. Woynarovich 1997-2000)
OTKA T030173. Theoretical study of magnetically or electrically low-dimensional models (J. Sólyom, 1999-2002)
MAKA[2] JF 555/95-B Unconventional behavior of low-dimensional magnetic and electric systems (J. Sólyom, 1996-1999)

Publications

Articles

A.1. I. Peschel*, M. Kaulke*, Ö. Legeza: Density matrix spectra for integrable models. *Annalen der Physik* **8**, 153-164 (1999)

A.2. Ö. Legeza and J. Sólyom: Response of finite spin-S Heisenberg chains to local perturbations. *Phys. Rev. B* **59**, 3606-3611 (1999)

A.3. E.H.Kim* and J.Sólyom: Opening of the Haldane gap in anisotropic two- and four-leg spin ladders. *Phys. Rev. B* **60**, (1999); *cond-mat*/9903241

A.4. M. Dudzinski*, G. Fáth, and J. Snajd*: Magnetic and quadrupolar order in a one-dimensional ferromagnet with cubic crystal-field anisotropy. *Phys. Rev. B* **59**, 13764-13774 (1999)

A.5. F. Woynarovich and P. Forgács*: Scaling limit of the one-dimensional attractive Hubbard model: The non-half-filled band case. *Nucl. Phys. B* **538** [FS] 701-730 (1999)

A.6. P. Millet*, C. Satto*, J. Bonvoisin*, B. Normand*, K. Penc, M. Albrecht* and F. Mila*: Magnetic properties of the coupled ladder system MgV_2O_5. *Phys. Rev. B* **57**, 5005-5008 (1998)

A.7. R. Neudert*, M. Knupfer*, M. S. Golden*, J. Fink*, W. Stephan*, K. Penc, N. Motoyama*, H. Eisaki* and S. Uchida*: Manifestation of spin-charge separation in the dynamic dielectric response of one--dimensional Sr_2CuO_3. *Phys. Rev. Lett*. **81**, 657-660 (1998)

A.8. G. Fáth, Z. Domanski*: Avalanche of bifurcations and hysteresis in a model of cellular differentiation. *Phys. Rev. E* **60**, 4604-4609 (1999)

[1] OTKA = Hungarian Scientific Research Fund

[2] MAKA = US-Hungarian Joint Fund

A.9. G. Bouzerar*, Ö. Legeza and T. Ziman*: Minimal model to describe the magnetism of $CuGeO_3$. *cond-mat*/9909375, *Phys. Rev. B*, accepted for publication

A.10. T. Hauer*, A. Rákos, F. Woynarovich: Scaling limit of the one-dimensional XXZ Heisenberg chain with easy axis anisotropy. *cond-mat*/9901184, *Nuclear Physics B*, accepted for publication

A.11. K. Penc and R. Lacaze*: spl(2,1) dynamical supersymmetry and suppression of ferromagnetism in flat band double-exchange models. *Europhysics Letters*, accepted for publication

A.12. S. B. Haley*, H. J. Fink*, G. Fáth: Internally orthogonal and tracking solutions of the Ginzburg-Landau and Schrödinger equations. *Phys. Rev. B*, accepted for publication

Conference Proceeding

A.13. E. H. Kim* and J. Sólyom: Evolution of the Haldane gap in anisotropic spin ladders. In: *Proc. Physical Phenomena at High Magnetic Field - III, Florida, 1999*, World Scientific Publishing Co. Inc., Singapore (1999)

Others

A.14. F. Woynarovich: On the symmetry of excitations in SU(2) Bethe Ansatz systems. *cond-mat*/9812415

A.15. G. Mihály, I. Kézsmárki*, F. Zámborszky*, M. Miljak*, K. Penc, P. Fazekas, H. Berger*, L. Forró*: Orbitally Driven Spin Pairing in the 3D Non-Magnetic Mott Insulator $BaVS_3$: Evidence from Single Crystal Studies. *cond-mat*/9911122

B. COMPLEX SYSTEMS

N. Menyhárd, F. Iglói, R. Juhász[+], 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 the Brownian motion of a classical particle in one-dimensional inhomogeneous environments where the transition probabilities follow random or aperiodic distributions. We found that the diffusion is generally anomalous: either the diffusion exponent is smaller than one, or the diffusion takes place in logarithmic time-scales. First passage time and persistence properties are also calculated analytically.

We have studied random quantum magnets when the distribution of the couplings and/or fields is either inhomogeneous or correlated. In one-dimensions we have obtained several exact results, which show that the critical and Griffiths-McCoy singularities are generally enhanced by such type of relevant perturbations.

Further - mainly numerical -investigations have been carried out in one-dimensional nonequilibrium systems from the point of view critical properties at directed-percolation-like phase transitions.

Quantum systems. — Semiclassical quantization has been derived for spins of not too small a quantum number $S > 5$. The $2S+1$ eigenvalues of a Hamiltonian, exhibiting resonant tunneling as the magnetic field parallel to the anisotropy axis increases, have been computed. Special attention has been paid to the resonance condition.

Using a new procedure we have determined the excitation energies of a degenerate Bose-gas in a magnetic trap in a wide range of the temperature and the potential anisotropy.

Other topics. — We have shown that the transient chaos has much reacher possibilities comparing to the permanent chaos, since there is a continuum of conditional measures even for a given dynamics. Its effect to the transient diffusion has also been determined.

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Grants:

OTKA T023642	Phase transitions in quasi-crystals, aperiodic and disordered systems (F. Iglói, 1997-2000)
OTKA T023791	Nonequilibrium phase transitions (N. Menyhárd, 1997-2000)
OTKA T030543	Mathematical study of systems of quantum spins and particles (A. Sütő, 1999-2002)

[+] Permanent position: Eötvös Loránd University, Budapest

Publications

Articles

B.1. F. Iglói and E. Carlon*: Boundary and Bulk Phase Transitions in the Two-dimensional Q>4 state Potts model. *Phys. Rev. B* **59**, 3783-3792 (1999)

B.2. F. Iglói, L. Turban* and H. Rieger*: Anomalous Diffusion in Aperiodic Environments. *Phys. Rev. E* **59**, 1465-1474 (1999)

B.3. H. Rieger* and F. Iglói: Average Persistence in Random Walks. *Europhys. Lett.* **45**, 673-679 (1999)

B.4. F. Szalma* and F. Iglói: Two-dimensional Dilute Ising Models: Critical Behavior Near Defect Lines. *J. Stat. Phys.* **95**, 763-770 (1999)

B.5. F. Iglói, R. Juhász and H. Rieger*: Griffiths-McCoy singularities in the Random Transverse-Field Ising Spin Chain. *Phys. Rev. B* **59**, 11308-11314 (1999)

B.6. E. Carlon*, F. Iglói, W. Selke* and F. Szalma*: Interfacial Adsorption in Two-dimensional Potts models. *J. Stat. Phys.* **96**, 531-540 (1999)

B.7. D. Karevski*, R. Juhász, L. Turban* and F. Iglói: Transverse-field Ising spin chain with inhomogeneous disorder. *Phys. Rev. B* **60**, 4195-4204 (1999)

B.8. L. Turban*, D. Karevski* and F. Iglói: Extended surface disorder in the quantum Ising chain. *J. Phys. A* **32**, 3907-3918 (1999)

B.9. H. Rieger* and F. Iglói: Random quantum magnets with long-range correlated disorder: Enhancement of critical and Griffiths-McCoy singularities. *Phys. Rev. Lett.* **83**, 3741-3744 (1999)

B.10. J.L. van Hemmen* and A. Sütő: Semiclassical quantization and resonance in spin tunnelling. *J. Phys. A: Math. Gen.* **31,** 0029-10043 (1998) and **32,** 4321 (1999)

B.11. J. Reidl*, A. Csordás*, R. Graham* and P.Szépfalusy: Finite temperature excitations of Bose gases in anisotropic traps. *Phys.Rev. A* **59,** 3816-3822 (1999)

B.12. N. Menyhárd and G. Ódor*: Nonequilibrium Kinetic Ising Models - Phase Transitions and Universality Classes in 1d. *Brasilian Journal of Physics,* accepted for publication

B.13. Z. Kaufmann*, A. Németh*, P. Szépfalusy: Critical States of Transient Chaos. *Phys. Rev. E,* accepted for publication

C. ELECTRONIC STATES IN SOLIDS

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

We have prepared a review article on the energetics of metal surfaces including our earlier studies about the **surface**, **step** and **kink energies** of mono-atomic surfaces. We have studied the stability of fcc (110) surfaces of some transition and noble metals in detail. Furthermore we have developed an efficient and accurate method to calculate the total energies of bulk metals and surfaces based on the **exact muffin-tin orbitals (EMTO) theory** developed by O.K. Andersen et al. The EMTO theory can be considered as an improved screened KKR (Korringa-Kohn-Rostoker) method which is able to treat large overlapping potential spheres. In our implementation of the EMTO theory the one electron equations are solved exactly using the Green's function formalism, and the Poisson's equation is solved within the spherical cell approximation. To demonstrate the accuracy of the method test calculations have been carried out.

The Airy Gas model of the edge electron gas developed by W. Kohn and A.E. Mattsson has been used to derive explicit density-dependent **kinetic and exchange energy functionals**. In this description the energy density becomes accurate where the curvature of the effective potential is negligible, and the total energies are systematically improved over the conventional local density approximation. The moderate impact of our gradient correction to the local density approximation in many cases brings the theoretical results to closer agreement with the experimental data than those obtained from the generalised gradient approximation.

Previously we implemented the so-called Abrikosov boundary condition in the **Locally Selfconsistent Multiple Scattering theory**. Now we carried the idea one step further, and formulated the theory named **Polymorphous Coherent Potential Approximation**. The conventional Coherent Potential Approximation is a very successful theory of the electronic structure of random substitutional alloys. However, it was well known, that it has defections treating charge transfers and related quantities. The new PCPA theory is designed to keep or further enhance all features of the conventional CPA theory and allow a proper treatment of the charge transfers. The success of the new theory has been demonstrated in CuZn and CuPd alloys.

We also studied the **Exchange Coupling** trough alloys spacers, where we generalised our previous theory for pure metals to include random substitutional binary alloys. We found, that just as in pure metals, the periods of oscillations are determined by the extremal nesting vectors of the Fermi surface. However, there is an additional exponential decay, which is determined by the coherence length at the particular point of the Fermi surface where the nesting vectors are.

The three-dimensional **transition metal compound** $BaVS_3$ which was studied in co-operation with experimentalists from the Technical University of Budapest, Zagreb, and the EPFL Lausanne, offers a unique collection of exotic features: **Mott transition** unaccompanied by magnetic order or static distortion; a low-temperature phase transition whose order parameter eludes identification; non-Fermi-liquid behaviour under pressure. Using a $3d^1$-based model for spin and orbital interactions, we started to develop a coherent picture of the observed phenomena. The intermediate insulating

[+] Permanent position: Technical University Budapest

state is described as a classical liquid of valence bonds which arises from thermal averaging over an exponentially large number of effective valence bond solid Hamiltonians.

In the field of high temperature superconductors we finished the interpretation of the Raman scattering data in the high-T_c superconductors, and have concluded that the appearance of the pseudogap in the underdoped samples is independent on the superconducting gap. In spite of the different mechanism, the obtained Raman relaxation rates coincide with the infrared relaxation rates.

Considering the relation between the electron-phonon coupling and transition temperature in YBCO and BSCCO samples we found that the data do not support theories based on phonon mechanism. Within the same model we described successfully the neutron scattering data in cuprates, and investigated vertex corrections to our Nested Fermi Liquid Theory applicable in the normal state..

Optical conductivity in **spin density waves** (SDW) attracted our attention due to a recent measurement with electric field perpendicular to the conducting chain direction. We calculated the frequency dependent conductivity in the presence of impurity scattering in SDW and found reasonable agreement with experiment. We also made the first steps towards building up the theory of **unconventional SDW** by working out the thermodynamics and some of the transport properties of this system.

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Levente Vitos	lv@power.szfki.kfki.hu

Grants

OTKA T020030	Interacting electrons in low dimensions (A. Virosztek, 1996-99)
OTKA T023390	Ab initio study of the structural stability of solids and surfaces (J. Kollár, 1997-2000)
OTKA T022609	Ab initio studies of magnetic thin films (B. Újfalussy, 1997-2000)
OTKA T025505	Competition of ferromagnetism with other collective phenomena in the lattice models for electrons (P. Fazekas, 1998-2001)
OTKA T019045	Collective excitations in unconventional superconductors (I. Tüttő, 1997-1999)
TÉT[3] D52/96	Raman scattering in unconventional superconductors (I. Tüttő, 1997-1999)

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

AKP 98-66	Orbital ordering of electrons in magnetic materials (P. Fazekas, 1999-2000)

[3] Intergovernmental Science and Technics Project

Publications

Articles

C.1. A. Virosztek and J. Ruvalds*: Susceptibility scaling and vertex corrections for a Nested Fermi Liquid, *Phys. Rev. B* **59**, 1324-1332 (1999)

C.2. T. P. Devereaux*, A. Virosztek and A. Zawadowski: Neutron scattering and the B_{1g} phonon in the cuprates, *Phys. Rev. B* **59**, 14618-14623 (1999)

C.3. A. Virosztek, B. Dóra* and K. Maki*: Impurity scattering and frequency dependent conductivity in spin density waves, *Europhys. Lett.* **47**, 358-363 (1999)

C.4. V. Vescoli*, L. Degiorgi*, M. Dressel*, A. Schwartz*, W. Henderson*, B. Alavi*, G. Grüner*, J. Brinckmann* and A. Virosztek: Spin density wave gap in the Bechgaard salts $(TMTSF)_2X$, *Phys. Rev. B* **60**, 8019-8027 (1999)

C.5. M. Opel*, R. Hackl*, T. P. Devereaux*, A. Virosztek*, A. Zawadowski*, A. Erb*, E. Walker*, H. Berger* and L. Forró*: Physical origin of the buckling in CuO_2: electron-phonon coupling and Raman spectra, *Phys. Rev. B* **60**, 9836-9844 (1999)

C.6. B. Újfalussy, G.M. Stocks*, Xindong Wang*, D.M.C. Nicholson*, W.A. Shelton*, Yang Wang*, and B.L. Győrffy*: Constrained density functional theory for first principles spin-dynamics, *Journal of Applied Physics* **85**, 4824 (1999)

C.7. L. Vitos, H.L. Skriver*, J. Kollár: The formation energy for steps and kinks on cubic transition metal surfaces, *Surface Science* **425**, 212-223 (1999)

C.8. J. Kollár, L. Vitos, B. Johansson*, H.L. Skriver*: Metal surfaces: surface, step and kink formation energies, *Physica Status Solidi* (6) **217**, No.1. (1999)

C.9. M. Opel*, R. Nemetschek*, C. Hoffman*, R. Philipp*, F.P. Müller*, R. Hackl*, I. Tüttő, A. Erb*, B. Revaz*, E.Walker*, H. Berger*, L. Forró*: Carrier relaxation, pseudogap and superconducting gap in high-T cuprates: A Raman scattering study. *cond-mat*/9908208, *Phys. Rev. B,* accepted for publication

C.10. M. Opel*, R. Nemetschek*, F. Venturini*, R. Hackl*, I, Tüttő, H. Berger, L. Forró*, A. Erb*, B. Revaz* and E. Walker*: A light scattering study of dynamical carrier properties in cuprate systems, *Ferroelectrics*, accepted for publication.

C.11. L. Vitos, H.L. Skriver*, B. Johansson*, J.Kollár: Application of the exact muffin-tin orbitals theory: the spherical cell approximation, *Comp. Mat. Science*, accepted for publication

C.12. L. Vitos, B. Johansson*, H.L. Skriver*, J. Kollár: Stability of fcc(110) transition and noble metal surfaces, *Comp. Mat. Science*, accepted for publication

C.13. L. Vitos, B. Johansson*, J. Kollár, H.L. Skriver*: The local kinetic energy density of the Airy Gas. *Phys. Rev. A*, accepted for publication

C.14. B. Dóra*, A. Virosztek and K. Maki*: The optical conductivity in spin density waves. *J. Physique*, accepted for publication

C.15. B. Dóra* and A. Virosztek: Unconventional spin density waves in quasi one-dimensional systems *J. Physique*, accepted for publication

C.16. A. Virosztek, B. Dóra* and K. Maki*: Microwave conductivity in spin density waves. *Ferroelectrics*, accepted for publication

Book, bookchapter

C.17. P. Fazekas: Lecture Notes on Electron Correlation and Magnetism, *Series in Modern Condensed Matter Physics*, Vol. 5, pp. 1-777, World Scientific, Singapore, 1999.

C.18. J. Kollár, L. Vitos, H.L. Skriver*: From the ASA towards the full potential *Lecture Notes in Physics*, Springer Series, pp.1-28, accepted for publication

Other

C19. G. Mihály*, I. Kézsmárki*, F. Zámborszky*, M. Miljak*, K. Penc, P. Fazekas, H. Berger* and L. Forró*: Orbitally Driven Spin Pairing in the 3D Non-Magnetic Mott Insulator $BaVS_3$: Evidence from Single Crystal Studies, *cond-mat*/9911122.

D. NON-EQUILIBRIUM ALLOYS

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

Structure and magnetic properties of nanocrystalline soft magnets. — Nanocrystalline $Fe_{92-x}Zr_7B_xCu_1$ ($2 \le x \le 23$) alloys were prepared by a heat treatment up to the first crystalline stage of the amorphous ribbons. The nanocrystalline state and the grain sizes of the nanosize ferromagnetic *bcc* precipitates embedded in the ferromagnetic residual amorphous matrix were determined by X-ray diffraction. ^{57}Fe Mössbauer spectroscopy was used to estimate the relative amount of Fe in the *bcc* phase. The combination of the *bcc* grain size and the quantity of the *bcc* phase allows the determination of the characteristic thickness of the residual amorphous phase which was found to be about 4 nm, independent of composition. The iron content of the residual amorphous phase was estimated to be about 67 at.% from the amount of the precipitated *bcc* phase determined from the Mössbauer measurements.

The Curie temperature of the residual amorphous phase, ^aT_c is determined in this two phase-system by Mössbauer spectroscopy via the extrapolation of the temperature dependence of its hyperfine field. An unusual composition dependence was found with a minimum around x=12, the increase of the Curie temperature has reached about 200 K both for decreasing and increasing Zr content (Fig. 1). This dependence is to be contrasted with the continuous decrease with increasing Zr content, expected and observed for the bulk-size amorphous alloys in good agreement with that of ^aT_c at high B concentrations. Since the characteristic thickness of the residual amorphous phase is composition independent, the unusual Zr-content dependence of the ^aT_c increase cannot be explained by the assumed penetration of the exchange interaction between the *bcc* granules. The anomalous increase of ^aT_c is attributed to magnetovolume effects.

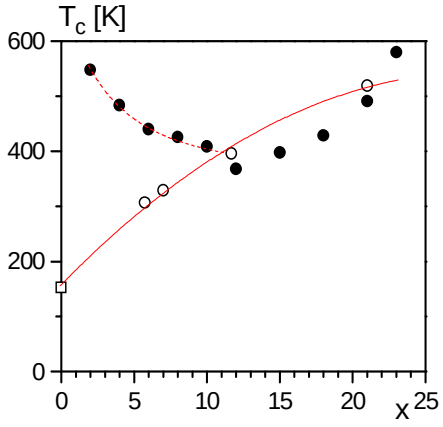

Fig. 1. *Curie temperature of the residual amorphous tissue of the $Fe_{92-x}Zr_7B_xCu_1$ nanocrystals (dots) together with that of melt-quenched $Fe_2(B_{1-y}Zr_y)$ amorphous alloys (empty circles, x=7(1-y)/y).*

In the B-rich region, between x=12 and 23 the width of the lines of the Mössbauer spectra of the *bcc* phase taken at high temperatures (i.e. above the Curie temperature of the residual amorphous phase) displayed significant reversible increase with increasing temperature: an obvious indication of magnetic relaxation (Fig.2). From the composition dependent starting temperature (400-600 K) to about 800 K the temperature dependence of the line broadening could be well approximated by an Arrhenius type expression which yields the magnetic anisotropy energy, E_{an} of the nanosize ferromagnetic grains. In the simplest superparamagnetic approximation the anisotropy energy is $E_{an}=KV$ (K is the uniaxial magnetic anisotropy constant, V is the volume of the relaxing particle). The superparamagnetic behaviour was verified also by magnetic measurements and the characteristic magnetic size of the relaxing particles was determined from the usual Langevin-type H/T plots.

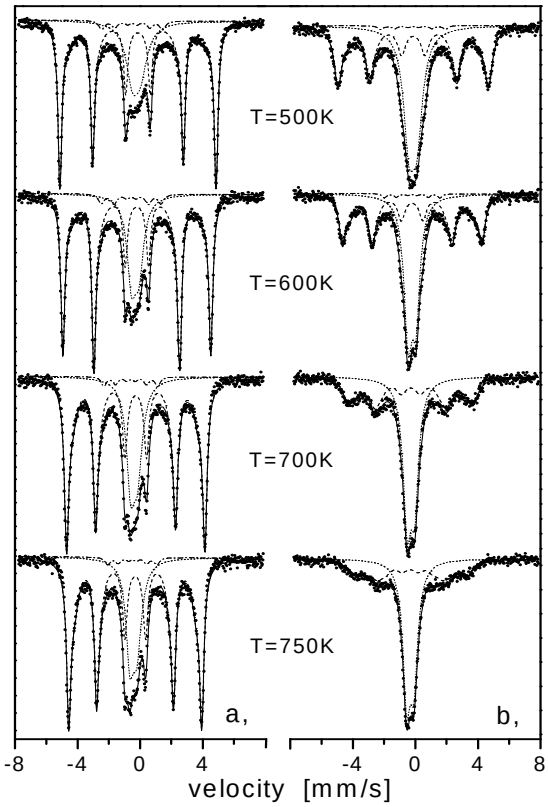

Fig. 2. *Temperature dependence of the Mössbauer spectra of the low B (x=4) and the high B (x=15) content* $Fe_{92-x}Zr_7B_xCu_1$ *nanocrystals, respectively. The separated components of the amorphous (dotted line), the interlayer (chain line) and the bcc (dashed line) are also shown.*

Grain boundary structure of iron. — Mössbauer spectra of different nanocrystalline samples are often interpreted according to the picture that they contain an extended grain-boundary region which is very different from that of the usual polycrystalline grain boundaries and has a significantly reduced density. However, increasing number of evidences are collected recently by high resolution transmission electron microscopy and X-ray fine structure measurements which confirm that significant structural disorder at the grain boundary extends no further than the planes immediately adjacent to the boundary plane. Therefore a critical review of the available Mössbauer data and a comparison of results obtained on samples prepared by different methods are important. Samples prepared by ball-milling of iron powder, partial crystallization of Fe-Zr-B-Cu amorphous ribbons and vacuum evaporation of Fe-B and Fe-Ag polycrystalline multilayers were examined and the Mössbauer spectra carefully analyzed as regarding possible impurities and chemical mixing at interfaces. These results set a limit to the difference between the hyperfine field of Fe atoms in the grain boundary region and in the bulk which is in the order of the linewidth and show that Mössbauer spectra of different nanocrystalline iron samples can be understood without supposing an extended region of the grain boundary with very distorted structure.

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Grants

OTKA T 020624	The photon- and electron-spectroscopic study of the interfaces of layer structures (J. Balogh, 1996-1999)
OTKA T 022413	The atomic and magnetic structure of nanosystems and interfaces (I. Vincze, 1997-1999)

OTKA F020092	The investigation of near-surface layers by spectroscopic and diffraction methods (D. Kaptás, 1996-1999)
OTKA T 030753	Magnetic systems with nanoscale inhomogeneities (I. Vincze, 1999-2002)
AKP 98-25 2,2	The relation of magnetic properties and the grain structure in nanocrystals (T. Kemény, 1999-2000)

Publications

Articles

D.1. D. Kaptás, T. Kemény, J. Balogh, L. Bujdosó, L.F. Kiss, T. Pusztai and I. Vincze: Magnetic properties of melt-quenched amorphous $Fe_2(B_{1-y}Zr_y)$ ($0 \leq y \leq 0.55$), *J. Phys.: Condens. Matter* **11,** L65-70 (1999).

D.2. T. Kemény, D. Kaptás, J. Balogh, L.F. Kiss, T. Pusztai and I. Vincze: Microscopic study of the magnetic coupling between nanoscale phases in a nanocrystalline soft magnet , J.*Phys.: Condens. Matter* **11,** 2841-2847 (1999) (see also E.13.)

D.3. J. Balogh, T. Kemény, I. Vincze, S. Szabó*, D. Beke* and J. Tóth*: Comment on the "Grain boundary structure and magnetic behavior in nanocrystalline ball-milled iron", *Phys. Rev*. **B59,** 14786-14787 (1999)

D.4. D. Kaptás, T. Kemény, J. Balogh, L. Bujdosó, L.F. Kiss, T. Pusztai and I. Vincze: Anomalous magnetic properties of the nano-size residual amorphous phase in nanocrystals, *J. Phys. Condens. Matter* **11,** L179-185 (1999)

D.5. S.C. Yu*, Y.Y. Song*, L.F. Kiss and I. Vincze: Study on the magnetic behavior of nanogranular $Cu_{80}Fe_{10}Co_{10}$ solid solution, *J. Magn. Magn. Mat.* **203,** 316-318 (1999)

D.6. J. Balogh, D. Kaptás, T. Kemény, I. Vincze and G. Radnóczi*: Comment on "Magnetically Ordered fcc Structure at the Relaxed Grain Boundaries of Pure Nanocrystalline Fe", *Phys. Rev. Letters* **82,** 4150 (1999)

D.7. J. Tóth, L.F. Kiss, E. Tóth-Kádár, A. Dinia*, V. Pierron-Bohnes* and I. Bakonyi: Giant magnetoresistance and magnetic properties of electrodeposited $Ni_{81}Cu_{19}$/Cu multilayers, *J. Magn. Magn. Mater*. **198-199,** 243-5 (1999) (see also I.8.)

D.8. A. Lovas, L.F. Kiss and I. Balogh: Low-temperature saturation magnetization and amorphous Curie point shift during the early stage of amorphous-nanocrystalline transformation, *J. Magn. Magn. Mat.*, accepted for publication (see also J.14.)

D.9. J. Balogh, L. Bujdosó, D. Kaptás, T. Kemény, I. Vincze, S. Szabó* and D.L. Beke*: Mössbauer Study of the Interface of Iron Nanocrystallites, *Phys. Rev.* **B**, accepted for publication

D.10. J. Balogh, L. Bujdosó, D. Kaptás, T. Kemény, I. Vincze, S. Szabó* and D.L. Beke*: Hyperfine field at grain boundary atoms in iron nanostructures, *Hyperfine Int.,* accepted for publication

D.11. T. Kemény, D. Kaptás, L.F. Kiss, T. Pusztai, J. Balogh and I. Vincze: The composition dependence of the structural and magnetic properties in $Fe_{92-x}Zr_7B_xCu_1$ nanocrystals. *J. Magn. Magn. Mat.,* accepted for publication

Conference Proceedings

D.12. K. Lázár*, L.F. Kiss, S. Pronier*, G. Onyestyák* and H.K. Beyer*: Iron nanoparticles in X and Y zeolites prepared by reduction with NaN_3, In: *Proc. NATO Advanced Research Workshop on Mössbauer Spectroscopy in Materials Science, Senec, Slovakia, 6-11 September 1998,* Mössbauer spectroscopy in materials science, NATO Science Series: 3. High Technology, Vol. 66, eds. M. Miglierini and D. Petridis (Kluwer Academic Publishers, London, 1999) pp. 291-8

D.13. A.R. Wildes*, N. Cowlam*, S. Al-Heniti*, L.F. Kiss and T. Kemény: A polarised neutron scattering study of two samples of $Fe_{90}Zr_{10}$. In: *Proc of the European Conference of Neutron Scattering, ECNS'99 (Budapest, 1-4 September 1999),* accepted for publication

E. X-RAY DIFFRACTION

G. Faigel, G. Bortel, L. Gránásy, Z. Jurek, K. Kamarás, G. Oszlányi, S. Pekker, T. Pusztai, M. Tegze

Fullerenes and their compounds. - The fullerenes are closed shell molecules containing only carbon atoms. The most abundant among them is the C_{60} molecule. Even in the simplest form (ie. solids of pure C_{60}) C_{60} is not fully understood. Illumination of the fcc pristine C_{60} by intensive light results in a phototransformation. This was the first case when intermolecular linkage of the fullerene molecules was proposed. Now it is well established that the bonding of C_{60} molecules in this material occurs through [2+2] cycloaddition. However, the structure of phototransformed C_{60} is not yet known. This is caused by two facts: first, photopolimerizations were done on thin films, therefore only very small amount of material is available for structural studies. Second, preliminary studies predict an inherent disorder in the bonding pattern of phototransformed C_{60}, which makes structural description difficult. To overcome the above problems we worked out a technique, which produces phototransformed C_{60} in bulk quantities. This allowed more precise x-ray powder diffraction studies and also differential scanning calorimetry measurements, which was not possible before. Based on the results of these measurements we suggested a structural model in which small closed oligomers (trimers and tetramers) build up the material.

Fullerenes can form a large variety of compounds with elements or other molecules. In the group of A_xC_{60} compounds (A=K, Rb, Cs x=1,3,4,6) there are materials with very interesting properties. Among them many superconducting materials (A_3C_{60}) with remarkably high critical temperature were found. Although the AE_xC_{60} type materials (AE=alkaline-earth metal) also show superconductivity, they are much less investigated. This is partly due to their more complicated structure and partly to the high melting point of the alkaline-earth metals, which makes the direct solid state chemical reaction problematic. We tried a simpler synthetic route to these compounds, the synthesis in liquid ammonia. As a test case we have chosen the Ca_4C_{60} composition, which is in the middle of a range where solid solution behavior with face centered cubic structure were reported. We found that a new $Ca_4(NH_3)C_{60}$ compound is formed by the inclusion of a single NH_3 molecule in the octahedral site of the fcc lattice. We expect that a series of compounds of this family can be synthetised.

X-ray holography with atomic resolution - In holography, the scattered radiation is mixed with a reference wave and the resulting interference pattern is recorded. The hologram contains both the intensity and the phase information and the 3 dimensional image of the object can be reconstructed. The most important limitation of this imaging technique is the spatial resolution, which is given by the wavelength and/or by the source size. Using x-rays for hologram forming and the atoms of the sample as sources or detectors atomic resolution can be achieved. We were the first to demonstrate experimentally the feasibility of x-ray holography with atomic resolution in 1996. To make this tecnique usable in practice further developments are necessary. First of all the data acquisition time has to be decreased. Therefore we implemented this method at synchroron sources. This resulted in measuring times in the range of 30 minutes. The second problem is the very anisotropic resolution in earlier measurements. We solved this by the extension of the hologram to the full

solid angle using the measured symmetry information of the Kossel and standing wave line patterns. An example is shown in Fig.1.

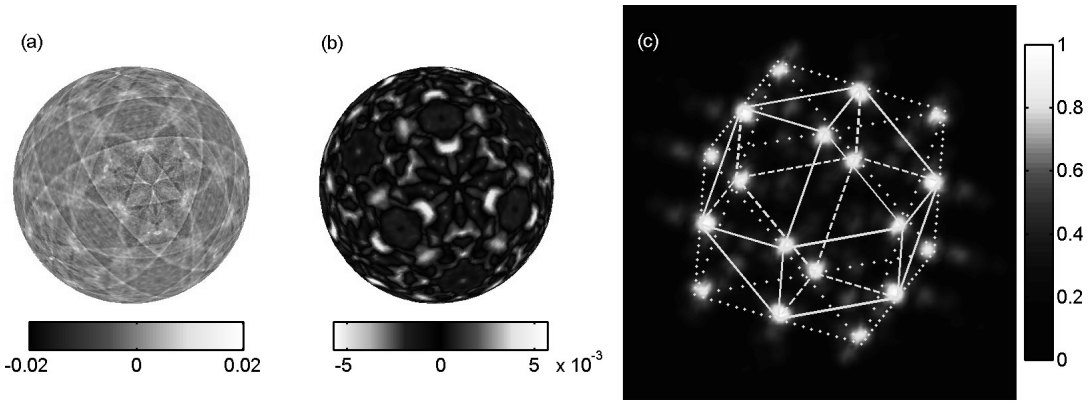

Fig.1. Standing wave pattern and holograms of a CoO sample(left panel). Reconstructed image of the Co atoms in 3D (right panel).

Theory of phase transformations. — We investigated crystal nucleation in various systems using cluster dynamics and continuum models, and crystal growth in the framework of the phase-field theory.

To clarify the mechanism of cross-interfacial molecular transport and the role of subcritical cluster population in determining the kinetics of crystal nucleation, cluster dynamics calculations based on viscosity-governed rate coefficients were confronted with experiments on crystal nucleation in stoichiometric oxide glasses. Systematic deviations have been observed in the temperature dependencies of the measured and predicted induction times that amount to orders of magnitude, and cannot be removed by considering the size-dependence of the interfacial free energy, the depletion of the monomers, or by enforcing the proper value of the free energy of monomers. Rather, it appears that while crystal nucleation and viscosity are both diffusion related processes, they are governed by different diffusion modes.

We calculated the free energy of ice nuclei and the nucleation rate in undercooled water in the framework of a single-order-parameter Cahn-Hilliard theory. The coefficients of the quartic free energy-order parameter relationship and of the square-gradient term were chosen so as to reproduce the measured Gibbs free energy difference, the ice/water interfacial free energy, and the interface thickness predicted by molecular dynamics simulations. Without adjustable parameters, the model reproduces fairly the experimental nucleation rates down to the deepest undercooling so far attained (~ –73 °C). The temperature and size-dependencies of the interfacial properties (free energy, Tolman-length, etc.) have been determined.

In cooperation with team H, we investigated the dynamic response of dendritic growth to time periodic forcing by modulated pressure and Joule heating in the framework of the phase-field theory. It has been shown that the dendritic morphology can be regularized in the typical frequency range of thermal dendritic side-branching. The experiments on liquid crystals support the predictions.

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Grants

OTKA F020027	X-ray studies of anisotropic and modulated structures (G. Oszlányi 1997-2000)
OTKA T022041	X-ray holography (M. Tegze, 1997-2000)
OTKA T025139	Theoretical investigation of the dynamics of nucleation and growth processes (L. Gránásy 1998-2001)
OTKA T029931	Structural studies of polymer fullerides (G. Faigel 1999-2002)
OTKA T019139	The study of polymer fullerides and other crystalline C_{60} compounds (S. Pekker1997-1999)
OMFB[4] 02264/98	New frontiers in structural biology (G. Faigel 1999-2000)
EU CT980377	New frontiers in structural biology (G. Faigel 1999-2000)

Publications

Articles

E.1. M.Tegze, G. Faigel, S. Marchesini*, M. Belakhovsky*, A.I. Chumakov*: Three dimensional imaging of atoms with isotropic 0.5 Å resolution, *Phys. Rev.Lett*. **82**, 4847-4851 (1999).

E.2. L. Gránásy: Nucleation: free energy of small clusters. (Invited for special issue.) *Int. J. Non-Equilibrium Processing*, **11**, 113-139 (1998).

E.3. L. Gránásy: Semiempirical van der Waals/Cahn-Hilliard theory: The size dependence of the Tolman-length. *J. Chem. Phys.* **109**, 9660-9663 (1998).

E.4. L. Gránásy, P.F. James*: Non-classical theory of crystal nucleation: Application to oxide glasses: Review. *J. Non-Cryst. Solids.* **253**, 210-230 (1999).

E.5. L. Gránásy, P.F. James*: Transient nucleation in oxide glasses: The effect of interface dynamics and subcritical cluster population. *J. Chem. Phys.* **111**, 737-749 (1999).

E.6. L. Gránásy: Cahn-Hilliard-type density functional calculations for homogeneous ice nucleation in undercooled water. (Invited contribution to the L.S. Bartell issue.) *J. Mol. Struct.* **485-486**, 523-536 (1999).

[4] National Commitee for Technological Development

E.7. L. Börzsönyi, T. Tóth-Katona, Á. Buka, L. Gránásy: Dendrites regularized by spatially homogeneous time-periodic forcing. *Phys. Rev. Lett.* **83**, 2853-2856 (1999). (See also H.3.)

E.8. T. Pusztai, G. Oszlányi, G. Faigel, K. Kamarás, L. Gránásy, S. Pekker: Bulk structure of phototransformed C_{60} , *Solid State Commun*. **111**, 595-599 (1999)

E.9. G. Faigel and M. Tegze: X-ray holography. *Report on Progress in Physics,* **62**, 355-392 (1999)

E.10. M.C. Miller*, G. Oszlányi, K.S. Ackroyd*, C. Marshall*, S.P. Collins*, D. Laundy*, R.J. Cernik*: PINCER: a portable data-acquisition program based on a command language interpreter, *J. Appl. Cryst.*, **31**, 972-973 (1998)

E.11. S.P. Collins*, B.M. Murphy*, C.C. Tang*, G. Oszlányi: SRS Station 16.3: description and utilization of a high-resolution diffraction facility. *J. Phys. D. Appl. Phys*. **32**, A81-A83, (1999)

E.12. V.C. Long*, J.L. Musfeldt*, K. Kamarás, A. Schilder*, W. Schütz*: Far-infrared study of the Jahn-Teller distorted C_{60} monoanion in C_{60} tetraphenylphosphoniumiodide. *Phys. Rev.* ***B*** **58**, 14338-14348 (1998)

E.13. T. Kemény, D. Kaptás, J. Balogh, L.F. Kiss.T.Pusztai, I. Vincze: Microscopic study of the magnetic coupling in nanocrystalline soft magnet. *J. Condens. Matter* **11**, 2841-2847, (1999) (See also D.2.)

E.14. V.C. Long*, J.L. Musfeldt*, K. Kamarás, A. Schilder*, W. Schütz*: Far-infrared study of C_{60}-tetraphenylphosphoniumiodide. *Synthetic Metals* **103**, 2435-2436 (1999).

E.15 G. Faigel: Holography with Resonant Quanta. *Hyperfine Interaction,* accepted for publication.

E.16. L. Gránásy, D.W. Oxtoby*: Cahn-Hilliard theory with triple-parabolic free energy: I. Nucleation and growth of a stable crystalline phase. *J. Chem. Phys*., accepted for publication.

E.17. L. Gránásy, D.W. Oxtoby*: Cahn-Hilliard theory with triple-parabolic free energy: II. Nucleation and growth in the presence of a metastable crystalline phase. *J. Chem. Phys*., accepted for publication.

Conference proceedings

E.18. T. Pusztai, G. Oszlányi, G. Faigel, K. Kamarás, L. Gránásy, S. Pekker: Structure of Phototransformed C_{60} revisited. In: *Proc. of XIII. International Winter School on the Electronic Properties of Novel Materials, 1999 Kirchberg Austria*, Eds. H. Kuzmany, J. Fink, M. Mehring and S. Roth, pp. 20-23

E.19. G. Oszlányi, S. Pekker, G. Faigel, L. Forró*: Structure of $Ca_4(NH_3)C_{60}$. In: *Proc. of XIII. International Winter School on the Electronic Properties of Novel Materials, 1999 Kirchberg Austria*, Eds. H. Kuzmany, J. Fink, M. Mehring and S. Roth, pp. 78-81.

E.20. S Pekker, J.-P. Salvetat*, E. Jakab*, J.-M. Bonnard*, L. Forró*: Chemical Functionalization of Carbon Nanotubes. In: *Proc. of XIII. International Winter School on the Electronic Properties of Novel Materials, 1999 Kirchberg Austria*, Eds. H. Kuzmany, J. Fink, M. Mehring and S. Roth, 1999, pp. 474-477.

E.21. D.M. Herlach*, W. Bender*, L. Gránásy, A. Garcia-Escorial*, A.L. Greer*, M. Kolb*, W. Kurz*, W. Löser*, A. Ludwig*, P.R. Sahm*, B. Vinet*: Undercooled melts: science, technology and application. In: *Proc. 2nd European Symp. on Utilization of the International Space Station ESTEC, Noordwijk, The Netherlands, 16 - 18 November 1998* (ESA SP-433, February 1999) pp. 315-322.

Others (technical digests, papers in Hungarian)

E.22 L. Gránásy, Nukleáció : A vírus kristályoktól a világegyetem szerkezetéig, (Nucleation: from virus crystals to the structure of the Universe, in Hungarian). In: *Lectures of the General Meeting 1999*, Hungarian Academy of Sciences, accepted for publication

E.23 G. Faigel: A röntgensugárzás hatása hétköznapjainkra (X-rays in our everyday life), Debreceni Szemle (1999) (in Hungarian), accepted for publication

F. ELECTRON CRYSTALS

G. Kriza, I. Pethes, P. Matus, G. Mihály[+]*, B. Sas*

Vortex motion in type-II superconductors. — The defining properties of superconductors are zero resistance and Meissner effect (i.e., the expulsion of magnetic field). Both may fail in Type-II superconductors where the magnetic field penetrates into the bulk in form of vortices and the motion of vortices may lead to dissipative transport. The understanding of the properties of the vortex system, therefore, is a fundamental problem in the physics of these superconductors. We have investigated the dissipative transport in the vortex glass state of the High-T_c superconductor $Bi_2Sr_2CaCu_2O_8$ using short current pulses. Field cooled preparation shows a higher critical current for dissipation than zero field cooled one but is metastable and convertible to the zero field cooled response by a small field excursion. The metastability appears on the low temperature side of a peak found in the temperature dependence of the critical current. We suggest that the onset of metastability signals a new thermodynamic ground state.

Nuclear magnetic relaxation in charge-density wave systems. — One of the specific predictions of the Bardeen-Cooper-Schrieffer theory of superconductivity was the existence of coherent electron-electron pairs manifested in so-called coherence effects such as the Hebel–Slichter anomaly in the nuclear spin-lattice relaxation rate. Such coherence effects have never been demonstrated in any other symmetry breaking ground state of the electronic system. We have found evidence of a quantum coherence peak in the temperature dependence of the ^{87}Rb NMR spin-lattice relaxation rate in the charge density wave system $Rb_{0.3}MoO_3$. The full exploitation of these results is under way.

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Grants

OTKA TO23786 NMR investigation of collective electronic states in organic conductors (G. Kriza, 1997-2000)

OTKA T029877: Vortex motion in type-II superconductors (G. Kriza, 1999-2001)

BALATON F-24/97 Periodic system in random field (B. Sas, 1998-1999)

French-Hungarian bilateral project TÉT F-24/97: Periodic systems in random potential (B. Sas, 1997-1999)

[+] Permanent position: Institute of Physics, Technical University, Budapest

Publications

Articles

F.1 G. Kriza, G. Szeghi*, I. Kézsmárki*, and G. Mihály: Field scaling and exponential temperature dependence of the magntoresistance in $(TMTSF)_2PF_6$. *Phys. Rev. B* **60**, R8434 (1999).

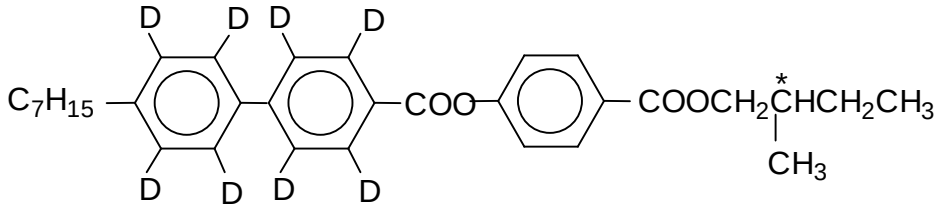
F.2 P. Matus, P. Bánki, and G. Kriza: ^{87}Rb NMR spin-lattice relaxation in the charge-density wave phase of $Rb_{0.3}MoO_3$. *J. Physique* IV **9**, Pr10-235 (1999)

F.3 B. Sas, F. Portier,* I. Pethes, K. Vad,* B. Keszei,* L. F. Kiss, I. Puha,* S. Mészáros,* and F. I. B. Williams*: Metastability line in the vortex phase of BSCCO. *J. Physique* IV **9**, Pr10-45 (1999)

G. LIQUID CRYSTAL RESEARCH

L. Bata, N. Éber, K. Fodor-Csorba, A. Jákli, E. Szabó, A. Vajda

Synthesis and properties of new liquid crystals. — A new synthetic pathway was developed for the preparation of isotope labeled (S)-(-)-4-[(2-methylbutyloxycarbonyl)phenyl-4-n-heptylbiphenyl carboxylate-d_8 (MBHB-d_8). In magnetic field a μSmC* subphase formed in the SmC* phase, where the orientational order dropped dramatically and increased again slowly with lowering the temperature. The proton analogue, MBHB, was prepared for electric polarization measurements and showed the same anomaly in the same temperature range. The unwounding of the helical structure and the change in the sign of the polarisation in the SmC* could explain the observed phenomenon.



MBHB-D_8

Dielectric spectroscopy measurements were carried out on the formerly synthesised deuterium labeled chiral ferroelectric monomeric and side chain polymeric liquid crystals.

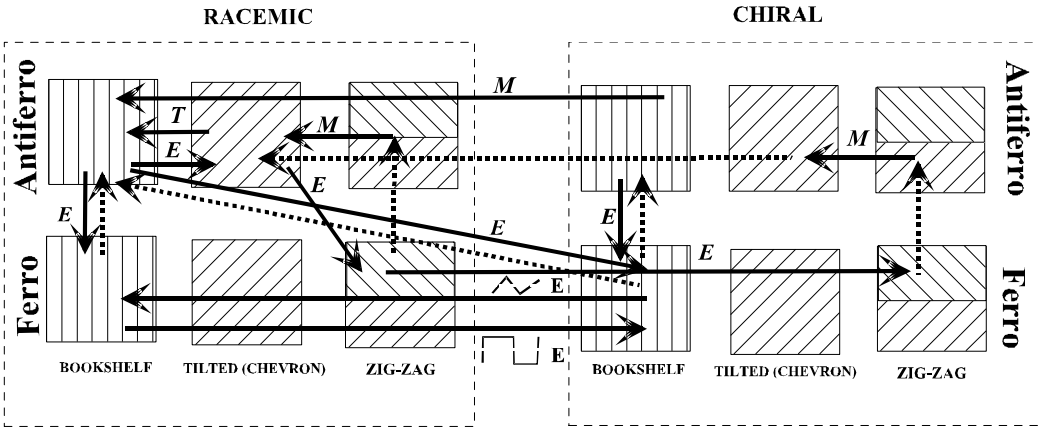
Achiral bent shaped cinnamic acid derivatives were prepared. The substituent effect on the mesophase behavior was investigated with the preparation of chlorine and methyl group containing derivatives. These groups were connected to the central ring, lowering the symmetry of the molecule and enhancing the mesophase formation ability.

Liquid crystals and their miscibility studies. — Four new chiral homologous series (DMn/m) S-(-)-4-(2-n-alkoxy-propionyloxy)biphenyl-4'-n-alkoxy-3,5-dimethylbenzoate having O-substituted S-(-)-lactic acid as terminal group were investigated by optical method. These LCs exhibited monotropic chiral smectic C and chiral nematic mesophases, and two of them blue phase as well. Binary mixtures of these compounds showed enantiotropic ferroelectric mesophases.

Structurally different chiral and non chiral binary and multicomponent mixtures having broad temperature range of enantiotropic ferroelectric mesophase were prepared for physical-electrooptical measurements. In order to understand more deeply the packing of the molecules in the mesophases of the mixtures, X-ray measurements were performed.

Study of ferroelectric liquid crystals. — Electro-optical and textural observations were carried out on a number of materials containing banana-shaped molecules. The voltage dependence of the net polarization indicated that the antiferroelectric ground state is weak, especially in the chiral domains. It was also observed that under long term application of strong fields a racemic state could be transformed to chiral. After field-removal the chiral state is metastable and the stable racemic structure recovers only slowly by a nucleation process that depends both on material parameters,

temperature and surface effects. The figure summarizes the morphological transitions observed in the B_2 phase of banana-shaped molecules.



Morphological transitions of the B_2 phase of banana-shaped molecules. Dashed arrows indicate relaxation processes. ***E*** *means electric field treatment,* ***M*** *stands for the mechanical shear and* ***T*** *means the temperature-induced process.*

Novel structures of liquid crystals. — Formation of coils is common in nature when achiral symmetry breaking occurs. Spectacular examples of single, double and triple coils were observed in smectic liquid crystal phases of achiral banana-shaped molecules. The number of observed left - and right-handed domains is equal reflecting the achiral nature of the constituent molecules. These studies indicate that the helical filaments consist of concentric smectic layers. The coiling stabilizes the growth process and suppresses the penetration of molecules from the isotropic phase, leading to moving of the tip with constant speed.

A polymorphism was observed in 4'-n-octyloxy 4-cyanobiphenyl (8OCB) which brings it into the line with the other homologues. Keeping the material between 35^{o}C and 38^{o}C after it was cooled from above the melting point of the stable crystal form (55^{o}C) regular platelets grow from usually one point and fill the whole sample. The texture is stable in room temperature for weeks. Upon heating it shows a melting point at 50^{o}C, i.e. 5 degrees below the stable crystalline melting point. It is interesting that all platelets are non-symmetric and have the same handedness.

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Grants:

OTKA T-020905 Deuterium labeling of liquid crystals (K. Fodor-Csorba, 1996-1999)

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

OTKA T-022772 Viscoelastic properties of smectic liquid crystals (N. Éber, 1997-2000)

OTKA T-023102 Investigation of physical properties of columnar and cubic mesophase (A. Jákli, 1997-2000)

OTKA F-029928 Synthesis of linear and bent core liquid crystals and study of their molecular geometry and mesophases (E. Szabó, 1999-2002)

ERBIC15CT960744 INCO Copernicus EC Research Network: Novel techniques and models for the surface treatment of liquid crystals with optical applications (A. Jákli, 1997-1999)

OMFB GB-75/96 Hungarian-British bilateral cooperation, New ferroelectric liquid crystals for displays (L. Bata, 1996-1999)

Volkswagen Stiftung with Iwan Stransky Institute, Berlin, Study of liquid crystals containing bent-core molecules (A. Jákli, 1998-1999)

Publications

Articles

G.1. A. Jákli: Electromechanical responses of antiferroelectric and ferrielectric liquid crystals. *J. Appl. Phys.* **85**, 1101-1104 (1999)

G.2. A. Jákli, Ch. Lischka*, W. Weissflog*, S. Rauch*, G. Heppke*: Layer structures of ferroelectric smectic liquid crystals formed by bent-core-molecules. *Mol. Cryst. Liq. Cryst.* **328**, 299-307 (1999)

G.3. T. Tóth Katona, N. Éber, Á. Buka: Thermally induced ageing in bicyclohexyl compounds and its influence on the N-SmB phase transition and interface morphology. *Mol.Cryst.Liq.Cryst.* **328**, 467-477 (1999) (see also H.4).

G.4. I. Jánossy, A. Jákli, G.G. Nair*, K.K. Kuldeep*, T. Kósa*: Optical Control of the alignment of a liquid crystal in the smectic A phase. *Mol. Cryst. Liq. Cryst.* **329**, 507-516 (1999) (see also H.6)

G.5. L. Calucci*, D. Catalano*, K. Fodor-Csorba, C. Forte*, C.A. Veracini*: Orientation, Structure and Dynamics in the Highly Ordered Smectic Phases of 7BEF5 by ^{2}H-NMR. *Mol. Cryst. Liq. Cryst.* **331**, 9-19, (1999)

G.6. M. Mertelj*, A. Jákli, M. Copic*: Dynamical behaviors of liquid crystals containing dispersed silica particles near SmA-N and N-I phase transitions. *Mol. Cryst. Liq. Cryst.* **331**, 81-87 (1999)

G.7. G. Pelzl*, S. Diele*, A. Jákli, Ch. Lischka*, I. Wirth*, W. Weissflog*: Helical superstructures in a novel smectic mesophase formed by achiral banan-shaped molecules. *Liquid Crystals* **26**, 135-139 (1999)

G.8. G. Pelzl*, S. Diele*, S. Grande*, A. Jákli, Ch. Lischka*, H. Kresse*, H. Schalmfuss*, I. Wirth*, W. Weissflog*: Structural and electrooptical investigations of the smectic phase of chlorine -substituted banana-shaped molecules. *Liquid Crystals* **26**, 401-413 (1999)

G.9. A. Jákli, M. Müller*, G. Heppke*: Rheology of a pyramidal liquid crystal. *Liquid Crystals* **26**, 945-952 (1999)

G.10. D.Z. Obadovic*, A. Vajda, M. Stancic*, K. Fodor-Csorba, L. Bata: The possibility of phase transition temperature shift in some ferroelectric liquid crystal mixtures. *J. of Res. in Physics* **68**, No.1, (1999).

G.11. A. Jákli, L. Almássy, S. Borbély, L. Rosta: Memory of silica aggregates dispersed in smectic liquid crystals: Effect of the interface properties. *The European Physical Journal B* **10**, 509-513 (1999) (see also K.2.)

G.12. D. Catalano*, E. Chiellini*, L. Chiezzi*, K. Fodor-Csorba, G. Galli*, E. Gács-Baitz*, S. Holly*, C.A. Veracini*: Partially deuterated side-chain liquid crystalline monomers and polymers: Characterization and order by ^{2}H NMR. *Mol. Cryst. Liq. Cryst.* accepted for publication.

G.13. G. Galli*, M.R. Di Bona*, K. Fodor-Csorba, B. Gallot*, E. Chiellini*: Synthesis and Mesophase Structure of Chiral Liquid Crystalline Polysiloxanes containing a New Phenylbenzoate Mesogen. *Mol. Cryst. Liq. Cryst.* accepted for publication.

G.14. F. Gouda*, A.A. Kutub*, K. Fodor-Csorba, G. Galli*, E. Chiellini*, L. Komitov*, J.P.F. Lagerwall*, S.T. Lagerwall*: Dielectric Investigations of a Chiral Monomer and Side Chain Polymer. *Mol. Cryst. Liq. Cryst.* accepted for publication.

G.15. D. Catalano*, M. Cifelli*, M. Geppi*, C.A. Veracini*, A. Jákli, K. Fodor-Csorba, E. Gács-Baitz*: Microscopic organization and tilt angle in smectic A and chiral smectic C phases: characterization and orientational order by ^{2}H NMR and electric polarization measurements. *Mol. Cryst. Liq. Cryst.* accepted for publication.

G.16. A. Vajda, M. Kaspar*, V. Hamplova*, P. Vanek*, K. Fodor-Csorba, L. Bata: Liquid Crystalline Properties of S-(-)-4-(2-n-alkoxy-propionyloxy)biphenyl-4'-n-alkoxy-3,5-dimethylbenzoate. *Mol. Cryst. Liq. Cryst.* accepted for publication.

G.17. D.Z. Obadovic*, A. Vajda, M. Stancic*, D. Lazar*, K. Fodor-Csorba, L. Bata: The investigations on some new liquid crystalline mixtures. *Mol. Cryst. Liq. Cryst.* accepted for publication.

G.18. A. Vajda, E. Szabó, A. Jákli, L. Bata, K. Fodor-Csorba: New Ferroelectric Mixtures of Liquid Crystalline α-Halogen Carboxylates. *Mol. Cryst. Liq. Cryst.* accepted for publication.

G19. N. Éber, A. G. Rossberg*, Á. Buka, L. Kramer*: New Scenarios in the Electroconvection of a Homeotropic Nematic Liquid Crystal. *Mol. Cryst. Liq. Cryst.* accepted for publication. (see also H.10)

G.20. M. Giocondo*, A. Jákli, A. Saupe*: Tilted smectic layers of a SmC* liquid crystal between homeotropically treated plates. *Eur. Phys. J. B*, accepted for publication.

G.21. G. Heppke*, A. Jákli, S. Rauch*, H. Sawade*: Electric field induced chiral separation in liquid crystals. *Phys. Rev. E.*, accepted for publication.

G.22. A.G. Rossberg*, N. Éber, Á. Buka, L. Kramer*: Abnormal Rolls and Regular Arrays of Disclinations in Homeotropic Electroconvection. *Phys. Rev. E Rapid Communication*, accepted for publication. (see also H.9)

Conference proceedings

G.23. D.Z. Obadovic*, A. Vajda, S. Jovanovic-Santa*, M. Stancic*, J. Petrovic*: The influence of new chiral additives on phase transitions of binary mixtures of some cholesteric liquid crystals. In: *Proc. of 6th European Powder Diffraction Conference, Budapest, Hungary,* Eds. R. Delhez and E.J. Mittemeijer, *Mat. Sci. Forum* (Trans Tech Publications, Switzerland), **321-324**, 1113-1118 (1999)

G.24. D.Z. Obadovic*, A. Vajda, M. Stancic*, D. Lazar*, K. Fodor-Csorba, L. Bata: The study of phase transitions of binary liquid crystalline mixtures. In: *Proc. of 6th European Powder Diffraction Conference, Budapest, Hungary,* Eds. R. Delhez and E.J. Mittemeijer, *Mat. Sci. Forum* **312-324**, 1131-1136 (1999) (Trans Tech Publications, Switzerland)

G.25. A. Jákli: Study of Liquid Crystal Composite Systems by Neutron Scattering. In: *Proceedings of the International School and Symposium on Small-Angle Neutron Scattering*, KFKI Report-1999-02/E

Others (papers in Hungarian, technical digests, reviews, etc.)

G.26. K. Fodor-Csorba, G. Galli*, C.A.Veracini*, D. Catalano*, L. Bata, S. Holly*, E. Gács-Baitz*, K. Újszászy*: Stabil izotóppal jelzett termotróp folyadékkristályok előállítása és vizsgálata II. (Synthesis and investigation of thermotropic liquid crystals labelled by stable isotopes II., in Hungarian) *Magyar Kémiai Folyóirat*, accepted for publication

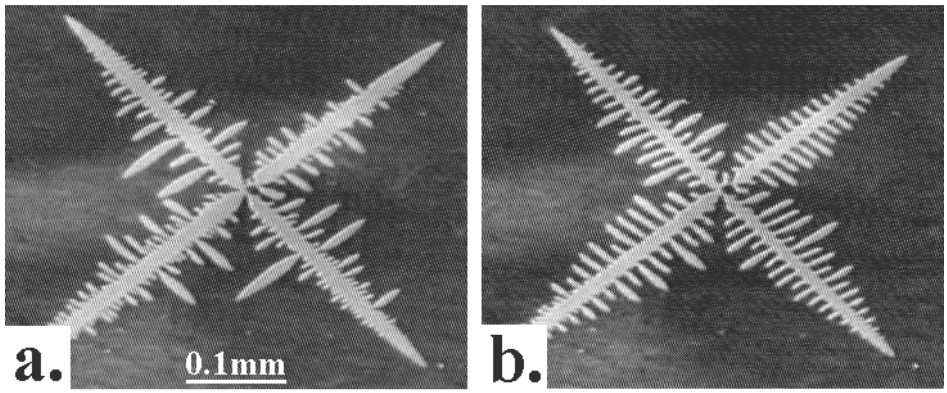
H. INSTABILITIES AND NONLINEAR PHENOMENA IN LIQUID CRYSTALS

Á. Buka, T. Börzsönyi, D. Goldschmidt, I. Jánossy, T. Tóth-Katona

Pattern formation:

– *Oscillatory shear induced instabilities:* The response of a homeotropically aligned nematic liquid crystal layer to oscillatory rectilinear shear has been measured for frequencies between 0.01Hz and 200Hz and layer thickness between 10μm and 130μm. The light transmission of the cell placed between crossed polarizers has been measured using a parallel light beam. Below the onset of the instability the experimental results for the transmitted light intensity agree quantitatively with numerical solutions of the nematodynamic eqations for different cell thicknesses, oscillation frequencies, and amplitudes. The critical oscillation amplitude for the onset of a spatial pattern could be reached for frequencies between 25Hz and 150Hz. The pattern consisted of stationary rolls perpendicular to the direction of the oscillation. The experimentally obtained frequency dependence of the critical shear amplitude for the roll instability for different cell thicknesses was compared with an existing theory and the results of numerical calculations [H1]. The optical response of the nematic liquid crystal confined between plates with strong homeotropic and weak planar anchoring (hybrid geometry) under oscillatory shear has been also measured. A critical shear amplitude has been found above which the director deviates from the planar orientation at the substrate with weak anchoring and the dependence of the tilt angle on the displacement amplitude has been obtained. The anchoring strength and surface viscosity for the SiO-evaporated substrate has been estimated [H5].

– *Nematic - smectic B interface:* Regularization of the dendritic side-branching has been achieved by spatially homogeneous time-periodic forcing, namely by pressure oscillations (see figure) and by modulated volumetric heat release both in numerical simulations (based on the phase-field model) and experimentally. To identify the range of conditions under which periodic external perturbations dominate the pattern formation, the parameter space defined by the frequency, the amplitude, and the waveform of the modulations, as well as by the undercooling and by the anisotropy of the system has been mapped [H3].



growth with inherent noise *growth with periodic forcing*

– *Viscous fingering:* Dendritic side-branching has been induced and/or regularized at the nematic – air interface by modulated electric field that influences the

effective viscosity of the nematic liquid crystal in the plane of observation. An upper modulation frequency of the regularization has been measured as a function of the driving force.

– *Electrohydrodynamic instabilities:* Unusual electroconvection scenarios have been found in a homeotropic nematic liquid crystal subjected to a small magnetic field such as: the existence of two Lifshitz frequencies, oscillations between pattern free state and chaos, as well as CRAZY rolls (a spatial period doubling phenomenon involving disclination loops). The variation of the azimuthal angle of the director has been measured around the normal roll - abnormal roll transition at various frequencies. This allowed the first quantitative verification of an amplitude description for a system with (nearly) spontaneously broken isotropy. With the same experimental technique a conclusive picture of the 3d director configuration in CRAZY rolls could also be obtained [H9].

– *Loop defects:* The experimentally observed loop line defect in nematic liquid crystals has been described. The critical size of the loop has been measured below which it spontaneously shrinks and transforms into a point defect. The experiment has been performed with 5CB which gives rise to twist disclinations as do most of the usual nematics. For this kind of disclination an in-plane force due to the boundary condition acts on the line and influences the critical radius. A model has been constructed which is in good agreement with experimental measurements and the line tension of the disclination has been deduced [H2].

Non-linear optics.

– *Laser-induced effects in liquid crystals:* The texture of a liquid crystal in the smectic A phase has been regulated with the help of a photosensitive substrate. It has been shown that the light-induced realignment of the director configuration can persist in a nematic – smectic A phase transition and can cause rearrangement of the smectic layers within the illuminated area. The ratio between the azimuthal anchoring strengths on the photosensitive and rubbed polyimide plates has been estimated [H6].

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Grants:

OTKA T-014957 Structure formation in non equilibrium, complex systems (Á. Buka, 1995-1999)

OTKA T-024098 Laser induced phenomena in smectic liquid crystals (I. Jánossy, 1997-2000)

OTKA F-022771 Interfacial patterns and convective instabilities (T. Tóth-Katona, 1997-2000)

OTKA N-31165, MTA-OTKA-NSF: Optical alignment of liquid crystals (I. Jánossy, 1999-2001)

ERB FMRX-CT 96-0085) EC Research Network: Pattern formation, noise and spatio- temporal chaos (Á. Buka, 1996-2000)

IC15-CT98-0806 Inco Copernicus: Photonic devices: new liquid crystalline composite materials (I. Jánossy, 1999-2001)

PST.CNS 975474 NATO Linkage Grant: Patterns and chaos in electroconvection of liquid crystals (Á. Buka, 1999-2000)

MTA-JSPS 39 (Hungarian-Japanese bilateral) Electrohydrodynamic instabilities and nonlinear phenomena in liquid crystals (Á. Buka, 1999-2001)

OMFB (TéT) F-2/98 (Hungarian-French bilateral) Instabilities and defect dynamics in liquid crystals (Á. Buka, 1999-2001)

Publications

Articles

H.1. T. Börzsönyi, Á. Buka, A.P. Krekhov* and L. Kramer*: Response of a homeotropic nematic liquid crystal to rectilinear shear. *Phys.Rev.* **E58**, 7419-7427 (1998)

H.2. S. Thiberge*, C. Chevallard*, Á. Buka and J.M.Gilli*: Critical radius of loop defects in a homeotropic nematic liquid crystal. *Liq. Cryst.* **26**, 1225-1234 (1999)

H.3. T. Börzsönyi, T. Tóth-Katona, Á. Buka and L. Gránásy: Dendrites regularized by spatially homogeneous time-periodic forcing. *Phys. Rev. Lett.* **83**, 2853-2856 (1999) (see also E.7.)

H.4. T. Tóth-Katona, N. Éber and Á. Buka: Thermally induced ageing in bicyclohexyl compounds and its influence on the N – SmB phase transition and interface morphology. *Mol. Cryst. Liq. Cryst.* **328**, 467-477 (1999) (see also G.3)

H.5. M.V. Khazimullin*, T. Börzsönyi, A.P. Krekhov* and Yu.A. Lebedev*: Orientational transition in nematic liquid crystal with hybrid alignment under oscillatory shear. *Mol. Cryst. Liq. Cryst.* **329**, 247-254 (1999)

H.6. I. Jánossy, A. Jákli, G.G. Nair*, K.K. Raina* and T. Kósa*: Optical control of a liquid crystal in the smectic A phase. *Mol. Cryst. Liq. Cryst.* **329**, 507-516 (1999) (see also G.4)

H.7. I. Jánossy: Optical reorientation in dye-doped liquid crystals. *Journ. Nonlinear Opt. Phys. Mater.* **8**, 361-377 (1999)

H.8. T. Tóth-Katona, T. Börzsönyi and Á. Buka: Pattern formation at the nematic smectic-B interface. *Mol. Cryst. Liq. Cryst.* accepted for publication

H.9. A.G. Rossberg*, N. Éber, Á. Buka and L. Kramer*: Abnormal rolls and regular arrays of disclinations in homeotropic electroconvection. *Phys. Rev. E*, Rapid Communication, accepted for publication (see also G.22)

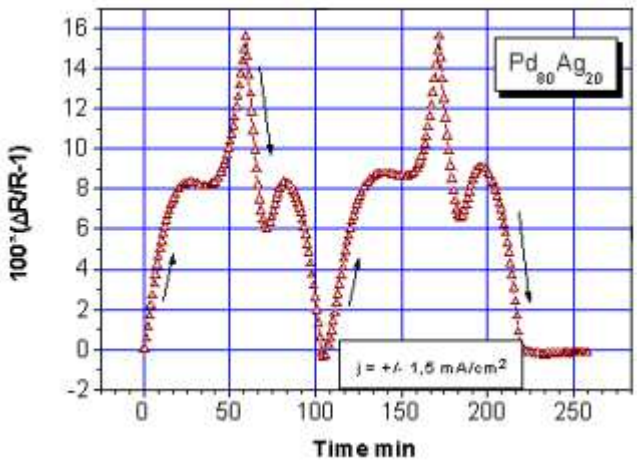
H.10. N. Éber, A.G. Rossberg*, Á. Buka and L. Kramer*: New scenarios in the electroconvection of a homeotropic nematic liquid crystal. *Mol. Cryst. Liq. Cryst.* accepted for publication (see also G.19)

I. METAL PHYSICS

K. Tompa, I. Bakonyi, M. Bokor[+] , J. Garaguly, Cs. Hargitai, Gy. Lasanda, T. Marek[++] , L. Péter, J. Tóth, E. Tóth-Kádár

Metal-hydrogen systems. **—** In the ^{1}H NMR study of $\mathbf{Zr_y(Ni_{1-x}Cu_x)_{1-y}-H}$ amorphous alloy-hydrogen systems, low-temperature ("rigid-lattice") spectrum shape and second moment (M_2), spin-lattice (T_1) and spin-spin (T_2) relaxation times have been measured and interpreted. The line shape can be described by the Harper-Barnes function with continuously changing exponent as a function of the hydrogen content. The second moment-hydrogen concentration data can be fitted by a power function of 3/4 exponent. These results show local fields originating from a few proton neighbours contrary to the "lattice gas"-like continuous hydrogen distribution. The interpretation of T_1 concludes to a strong paramagnetic contribution of unknown origin in the low temperature range. The careful analysis of the CPMG echo-train amplitude and T_2 demonstrates the partition of hydrogen into a diffusible and a trapped component in disordered systems, and the latter one correlates with the abundance probability of Zr-poor tetrahedra.

High-purity $\mathbf{Pd_{1-x}Ag_x}$ (x = 0.1; 0.2 and 0.35) alloy foils were prepared, charged with hydrogen, and in-situ-NMR spectrum, T_1 and T_2 relaxation times, electrical resistivity measurements were started on these fcc crystalline alloys, on model materials representing a chemically disordered system for the hydrogen storage. The resistivity measurements and the in-situ NMR study realised first in the world in a hydrogen storing metal give a unique chance for the investigation of non-equilibrium hydrogen charging, discharging and diffusion processes. Parallel charging experiments have been made on Pd-Ag alloys by the two commonly used methods, namely by the gaseous and electrolytic methods. Both kinds of experiment were carried out under non-equilibrium conditions.



The electrolytic method has the advantage that the charging-discharging (~anodic) process is reversible. The complete understanding of the non-monotonic time dependence seems to be a good challenge.

The resistivity change during two charging-discharging processes

Transition metal complexes. — Continuing the study of transition metal complexes, ^{1}H and ^{19}F NMR spectra and spin-lattice relaxation times were measured and interpreted in $[M(1\text{-R-}1H\text{-tetrazole})_6](BF_4)_2$ compounds (M = Fe or Zn; R = methyl or ethyl) between room temperature and 2.2 K. The characteristics of the reorientational

[+] *Ph.D. student (Eötvös University) supported also by the HAS and the Soros Foundation Hungary*

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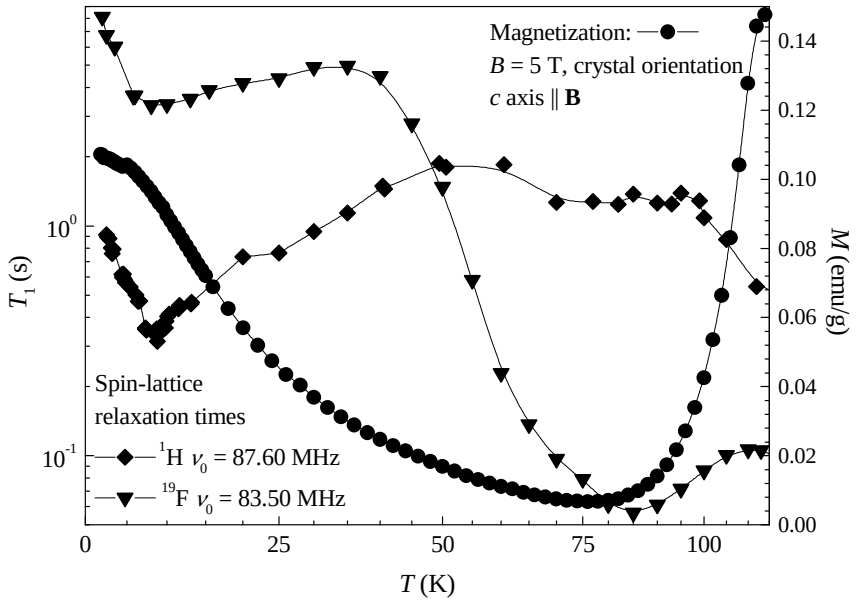
motions of the BF_4^- ions and the R groups and the relaxation due to the high-spin state FeII ions were evaluated and the results obtained were similar to those of the R = n-propyl compound. The unusual temperature dependence of ^1H and ^{19}F relaxation times of $[Fe(1\text{-n-propyl-1H-tetrazole})_6](BF_4)_2$ at T < 50 K (see the figure below) reflects the presence of FeII ions with $S \neq 0$ state. The sharp minima at ~9 K indicate interaction between them. The behaviour of the magnetization supports these assumptions.

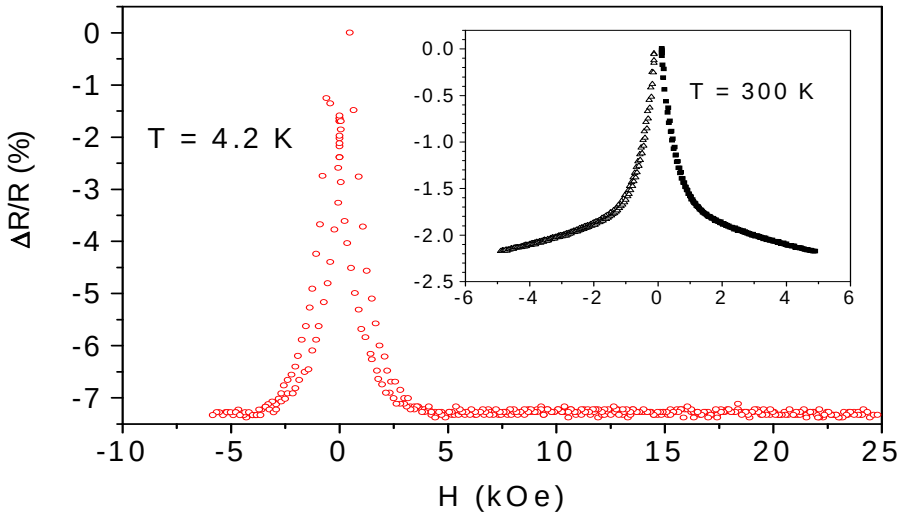


Unusual temperature dependence of ^1H and ^{19}F relaxation times and magnetization of $[Fe(1\text{-n-propyl-1H-tetrazole})_6](BF_4)_2$ at T < 50 K

Metastable metallic phases. — We have reported previously that a single-phase, fully nanocrystalline $Hf_{11}Ni_{89}$ alloy with the $HfNi_5$ structure could be produced by melt-quenching and now we describe the results of thermal stability studies of this phase. During a linear heating process of the nanocrystalline $Hf_{11}Ni_{89}$ alloy, two exothermal peaks can be observed by DSC. The first peak corresponds to a grain growth process and the second to a Ni precipitation in significant amounts. The microstructure evolution during a pre-annealing treatment performed well below the grain growth temperature was studied by X-ray diffraction and DSC. The observed changes could be mainly ascribed to a redistribution of the excess Ni atoms with respect to the stoichiometric composition. The thermal stability of the nanocrystalline samples was depressed evidently during the microstructure evolution characterized by lowered DSC peak temperatures and lowered activation energies corresponding to the two peaks. The microstructure analysis indicated that the crystallites and the interfacial regions approach to an equilibrium state during the preannelaing treatment. Therefore, the depressed thermal stability could be explained based on the fact that less atomic diffusion inside the crystallites is involved during the grain-growth process in the pre-annealed sample.

Metallic multilayers — We have studied the magnetic and magnetoresistance properties of electrodeposited $Ni_{81}Cu_{19}$(3nm)/Cu(d_{Cu}) multilayers where the Cu layer thickness d_{Cu} was varied from 0.5 nm to 3 nm and a bulk homogeneous $Ni_{81}Cu_{19}$ alloy electrodeposit. The room temperature magnetization indicated a deviation of the saturation magnetization of the multilayers from the expected saturation values

calculated by using the thicknesses of the magnetic and nonmagnetic sublayers. This was explained by assuming that there is a compositional variation across the magnetic/nonmagnetic interfaces. On the other hand, the room temperature magnetoresistance measurements revealed that all the multilayers with $d_{Cu} \geq 0.75$ nm exhibited giant magnetoresistance (GMR) and there was a maximum GMR around $d_{Cu} = 1$ nm. However, beyond the peak the GMR remained nearly constant up to $d_{Cu} = 3$ nm. From a comparison with the magnetizaton curves, it was suggested that this prevailing GMR component which is present in the magnetoresistance curves with a slope of about -0.6 %/kOe for H > 1 kOe (see insert in the figure below) may be connected with the presence of a compositional variation across the interfaces. Namely, some regions between the magnetic and nonmagnetic sublayers may have a composition close to the onset of para-ferromagnetic transition of Ni-Cu alloys and as such may exhibit superparamagnetic (SPM) behaviour. In contrast, low temperature magnetoresistance curves showed a saturation in magnetic fields as low as 4 kOe (as demonstrated in the figure below) whereas at room temperature, no saturation of the magnetoresistance measurements up to 18 kOe could be observed in some cases.



Magnetoresistance curves of an electrodeposited $Ni_{81}Cu_{19}$(3nm)/Cu(1nm) multilayer at T =4.2 K. The insert shows the same at T = 300 K.

Based on the composition variation at the interfaces, a model for the magnetization profile and the magnetization reversal at the magnetic/nonmagnetic interfaces can be suggested. It is argued that the existence of SPM regions in the interfaces can well explain the striking differences between the magnetoresistance curves at 300 K and 4.2 K. Namely, at sufficiently low temperatures, the SPM regions either themselves become ferromagnetic and can then be saturated around 4 kOe as the bulk Ni-Cu alloys or remain in the SPM state but can still be saturated at such low fields. Once all the magnetization saturated at 4 kOe and all the magnetic moments aligned parallel, an increase of the magnetic field is not expected to cause any further change in the resistance, at least in comparison with the size of the observed GMR at low fields. Electrochemical and GMR studies recently completed on electrodeposited Ni-Cu/Cu multilayers also gave strong evidence for the inevitable occurrence of a composition profile at the interfacas due to the pulse-plating technique commonly used in electrodeposition. However, other multilayer preparation methods may also result in

some intermixing at the interfaces and, as shown in the present work, a study of the temperature variation of the magnetoresistance curves may yield a further useful characterization of this intermixing.

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Grants

OTKA T016670 NMR relaxation and local properties in solids (K. Tompa, 1995-1999)

OTKA T 022 124 Preparation and investigation of single-phase nanocrystalline metals (I. Bakonyi, 1997-2000)

AKP 97-48 2,2/37 Hydrogen diffusion and chemical order in hydrogen storing Pd-Ag alloys (K. Tompa, 1998-1999)

OMFB TéT M-8/97: Magnetic domain imaging in nanocrystalline materials (Instituto Nacional de Investigaciones Nucleares, Mexico, 1998-2000; CONACYT)

OMFB TéT IND-7/97: Layered magnetic materials (Indian Association for the Cultivation of Science, Calcutta, India, 1998-1999; Ministry of Science and Technology of India)

HAS-INSA Project No. 7: Magnetic and transport properties of metastable phases and low-dimensional systems (Univ. of Hyderabad, India, 1998-2000)

HAS-CNRS Project No. 15: Microstructure, magnetic properties and magneto-resistance of metallic multilayers (Inst. de Physique et Chimie des Materiaux de Strasbourg, France, 1999-2000)

Publications

Articles

I.1. I. Bakonyi, Á. Cziráki*: Nanocrystalline-forming ability of alloys by melt-quenching. *Nanostruct. Mater.* **11**, 9-16 (1999)

I.2. I. Bakonyi, E. Tóth-Kádár, J. Tóth, T. Becsei*, T. Tarnóczi, P. Kamasa: Magnetic and electrical transport properties of electrodeposited Ni-Cu alloys and $Ni_{81}Cu_{19}$/Cu multilayers. *J. Phys. Cond. Matter* **11**, 963-973 (1999) (see also J.3)

I.3. Á. Cziráki*, I. Gerőcs*, L.K. Varga, A. Lovas, I. Bakonyi: Structural differences between the nanocrystalline $Fe_{86}Zr_7B_6Cu_1$ and $Fe_{73.5}Si_{13.5}B_9Nb_3Cu_1$ alloys. *Nanostruct. Mater.* **12**, 1109-1112 (1999) (see also J.4)

I.4. Á. Cziráki*, J.G. Zheng*, A. Michel*, Zs. Czigány*, G. Nabiyouni*, W. Schwarzacher*, E. Tóth-Kádár, I. Bakonyi: Cross-sectional transmission electron microscopy study of the microstructure of electrodeposited Co-Ni-Cu/Cu multilayers. *Z. Metallkde*. **90**, 278-283 (1999)

I.5. Z.F. Dong*, K. Lu* and I. Bakonyi: Influence of pre-annealing on the thermal stability of a nanocrystalline Hf-Ni alloy. *Nanostruct. Mater.* **11**, 187-194 (1999)

I.6. R. Lück*, Z.F. Dong*, M. Schieffer*, I. Bakonyi, K. Lu*: Mictrostructure identification of an interfacial phase in a melt-spun Hf-Ni nanocrystalline alloy. *Philos. Mag. B* **79**, 163-176 (1999)

I.7. Á. Révész*, J. Lendvai*, I. Bakonyi: Nanocrystallization studies of a melt-quenched $Ni_{81}P_{19}$ amorphous alloy. *Mater. Sci. Forum* **312-314**, 499-504 (1999)

I.8. J. Tóth, L.F. Kiss, E. Tóth-Kádár, A. Dinia*, V. Pierron-Bohnes*, I. Bakonyi: Giant magnetoresistance and magnetic properties of electrodeposited $Ni_{81}Cu_{19}$/Cu multilayers. *J. Magn. Magn. Mater.* **198-199**, 243-245 (1999) (see also D.7.)

I.9. A. Vértes*, K. Süvegh*, M. Bokor, A. Domján*, T. Marek, M. Klapper*, C.U. Chisholm*, M. El-Sharif*, K. Tompa, Zs. Nemes-Vetéssy*, K. Burger*: Frontiers of positron and positronium chemistry in condensed media. *J. Radioanal. Nucl. Chem.* **239**, 29-36 (1999)

I.10. M. Bokor, T. Marek, K. Tompa, P. Gütlich*, A. Vértes*: Dynamics of BF_4^- anion reorientation in the spin-crossover compound [Fe(1-*n*-propyl-1*H*-tetrazole)$_6$](BF_4)$_2$ and in its Zn^{II} analogue. *European Physical Journal D*, accepted for publication

I.11. T. Marek, M. Bokor, Gy. Lasanda, K. Tompa, L. Párkányi*, J. Buschmann*: Temperature dependence of solid state ^{1}H NMR line shapes and M_2 in polycrystalline BF_4^- salts of 1-Propyltetrazole Complexes of Iron(II) and Zinc(II). *J. Phys. Chem. Solids*, accepted for publication

I.12. Á. Révész*, J. Lendvai*, I. Bakonyi: Nanocrystallization studies of a melt-quenched $Ni_{81}P_{19}$ amorphous alloy. *Nanostruct. Mater.*, accepted for publication

I.13. G. Vértesy*, A. Gasparics*, Z. Vértesy*, E. Tóth-Kádár: Influence of the core material polishing on the fluxset sensor's operation. *J. Magn. Magn. Mater.*, accepted for publication

J. METALLURGY AND MAGNETISM

L.K. Varga, A. Kákay[+], P. Kamasa, G. Konczos, Gy. Kovács[++], A. Lovas[+++], J. Pádár, L. Pogány, F.I. Tóth, B. Varga[++++], I. Varga[+++++]

Soft magnetic nanocrystalline alloys. — Our main activity in 1999 was centered around the tasks of a NATO Science for Peace program aiming to prepare magnetic nanocomposites which offer soft magnetic materials for audio and radio frequencies. This program started in March this year. In the first half of the year, we have optimized the properties of Finemet type nanocrystalline alloys for applications as interface transformer cores in ISDN lines. This application-oriented research which will be finalized next year is based on fundamental research aiming to develop the best soft magnetic material in the possible largest frequency interval. We have determined the effective anisotropy in both Si and Zr based nanocrystalline alloys for their optimal annealed state. The experimental values were 280 J/m^3 and 500 J/m^3,respectively, instead of about 1-5 J/m^3 expected by random anisotropy model calculations. We have explained the excellent coercivity values of nanocrystalline alloys within the domain wall pinning theory and obtained the following formula:

$$H_c=0192\ (<K>/J_s)(\delta/L_{ex})(T_c^{cr}/T_c^{am})$$

where <K> is the measured anisotropy constant, δ is the width of the amorphous spacer, L_{ex} is the exchange length calculated with the measured <K>. The small H_c values could be estimated within a factor of 2 by the above formula in spite of the relatively large effective anisotropy constant found experimentally. We have developed a model to simulate the temperature evolution of the experimental data of the initial susceptibility in nanocrystalline alloys. It was shown that the Hopkinson peak of the initial susceptibility, which is progressively rounded off and displaced to lower temperatures as the nanocrystallization proceeds, can be perfectly described without assuming a broad distribution of Curie temperatures of the residual amorphous matrix. It is only necessary to take into account that even above the T_c of the amorphous matrix, the effective anisotropy does not fall to zero in the decoupled state due to the residual interaction between the bcc nanocrystallites which exhibit a higher Curie temperature.

In a search for single-phase nanocrystalline alloys, we have started a systematic investigation of high silicon content $Fe_{1-x}Si_x$ alloys with $15 < x < 50$ obtained by rapid quenching from the melt. We were able to extend the basically cubic structure up to 34 at.% Si, near to the hexagonal Fe_5Si_3 stoichiometric compound. The magnetic properties (saturation magnetization, M_s, Curie point, T_c, spin wave stiffness, D_{sp} and magnetic anisotropy, K) determined on these single-phase alloys in the composition range $25 < x < 34$ fill in an important gap in the literature of Fe-Si alloys. From theoretical considerations, a parabolic decrease of M_s versus x_{Si} was found in the basically cubic range ($0 < x < 34$) which fits quite well the experimental results.

[+] *Ph.D. student (Eötvös University) supported by the Ministry of Education*

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[+++] *Permanent position: Technical University of Budapest*

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Around 33 at.% Si, a metastable Fe-Si nanocrystalline phase was prepared with the B2 structure which exhibited good soft magnetic behaviour (saturation J_s=0.6 T, coercivity H_c~100 A/m, resistivity ρ=200 $\mu\Omega\cdot$cm). This brittle and easy-to-powderize material is a promising substitute for ferrite type cores.

Temperature-modulated thermomagnetometry. — The combination of thermal analysis with other measurement techniques is very fruitful for the interpretation of the behaviour of the investigated physical system during heating or cooling. In cooperation with the Technical University of Koszalin (Poland), a thermoanalyser apparatus has been developed and built which permits the following kinds of measurement: differential thermal analysis (DTA), thermal dilatometry (TD), and thermomagnetometry (TM). In the last year, the thermoanalyser was modified to have a new feature: temperature modulation. The importance of temperature-modulated DTA lies in the possibility of the deconvolution of the response of the analysed sample to the temperature modulation, which yields information on reversible effects. The modification extends the measurement capabilities to perform a simultaneous analysis of specific heat changes as well and enables the separation of reversible and irreversible processes during phase transitions. Besides thermal analysis, the temperature-modulated thermomagnetometry enables a more detailed observation of the crystallization processes even in amorphous alloys with a crystallization temperature higher than the Curie temperature. The method is significantly new and further potential applications are under study.

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Grants

OTKA T020891 Study of intracellular element distribution in soil microorganisms (L. Pogány, 1996-1999)

GE-TUNGSRAM: Contract for materials research by SEM (L. Pogány, 1999)

AGMI (Material Testing and Quality Control Co.): Contract for design and construction of eddy-current probe for non-destructive testing of high-pressure chemical reactor walls at Tisza Chemical Works (TVK) (P. Kamasa, 1999)

MTA SZBK (Biological Research Centre of Szeged, HAS): Contract for the reconstruction of laserbeam scanning electron microscope (P. Kamasa, 1999)

NATO Science for Peace Project 97/1930: Magnetic nanocomposites for transformer cores and magnetic refrigeration (L.K. Varga, 1999-2003)

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

Publications

Articles

J.1. P. Kamasa, P. Myśliński*, B. Varga, Z. Jurasz*: Investigation of the oxidation process in rod and foil iron samples by thermomagnetic measurements. *acta phys. slovaca* **48**, 857-860 (1998)

J.2. A. Sólyom*, P. Marko*, P. Petrovič*, D. Matisová*, G. Konczos: Rapidly quenched microcrystalline Fe-Si-Co alloys. *acta phys. slovaca* **48**, 711-714 (1998)

J.3. I. Bakonyi, E. Tóth-Kádár, J. Tóth, T. Becsei*, T. Tarnóczi, P. Kamasa: Magnetic and electrical transport properties of electrodeposited Ni-Cu alloys and $Ni_{81}Cu_{19}$/Cu multilayers. *J. Phys. Cond. Matter* **11**, 963-973 (1999) (see also I.2.)

J.4. Á. Cziráki*, I. Gerőcs*, L.K. Varga, A. Lovas, I. Bakonyi: Structural differences between the nanocrystalline $Fe_{86}Zr_7B_6Cu_1$ and $Fe_{73.5}Si_{13.5}B_9Nb_3Cu_1$ alloys. *Nanostruct. Mater.* 12, 1109-1112 (1999) (see also I.3.)

J.5. D. García*, G.V. Kurlyandskaya*, M. Vázquez*, F.I. Tóth, L.K. Varga: Influence of field annealing on the hysteretic behaviour of the giant magneto-impedance effect of Cu wires covered with $Ni_{80}Fe_{20}$ outer shells. *J. Magn. Magn. Mater.* **203**, 208-210 (1999)

J.6. P. Kamasa, P. Myśliński*: Study of the thermal effects during microstructural changes of metastable alloys by means of temperature-modulated thermomagnetometry. *Thermochimica Acta* **337**, 51-54 (1999)

J.7. K. Lázár*, H.K. Beuer*, G. Onyestyák*, B.J. Jönsson*, L.K. Varga, S. Pronier*: Iron nanoparticles in X and Y zeolites. *Nanostruct. Mater.* **12**, 155-158 (1999)

J.8. V.T. Lebedev*, G.P. Gordeev*, A.I. Sibilev*, V.V. Klyubin*, Gy. Török, L. Cser, Gy. Káli, L.K. Varga, A. Brulet*: Neutron spin echo study of low-T_c ferrofluid. *J. Magn. Magn. Mater.* **201**, 80-83 (1999) (see also K.13.)

J.9. P. Myśliński*, P. Kamasa, J. Vandlik*: Analysis of alloys using DTA and TD methods with simultaneous thermomagnetic studies. *J. Therm. Anal. Calorim.* **56**, 233-238 (1999)

J.10. L. Takács*, A. Mossion*, K. Lázár*, L.K. Varga, M. Pardavi-Horváth*, A. Bakhshai*: ZnO-Fe nanocomposites via ball milling and annealing. *Nanostruct. Mater.* **12**, 245-248 (1999)

J.11. L.K. Varga, K.V. Rao*: Thermomagnetic study of metastable nanograin in soft magnetic nanocrystalline alloys. *Nanostruct. Mater.* **12**, 1157-1160 (1999)

J.12. V. Franco*, C.F. Conde*, A. Conde*, B. Varga, A. Lovas: Thermomagnetic study of $Fe_{73.5-x}Cr_xSi_{13.5}B_9Cu_1Nb_3$ (x=1, 3, 5, 10) alloys. *J. Magn. Magn. Mater.*, accepted for publication

J.13. S.N. Kane*, S. Sarabhai*, A. Gupta*, L.K. Varga, T. Kulik*: Effect of quenching rate on crystallization in $Fe_{73.5}Si_{13.5}B_9Cu_1Nb_3$ alloys. *J. Magn. Magn. Mater.*, accepted for publication

J.14. A. Lovas, L.F. Kiss, I. Balogh: Low-temperature saturation magnetization in the early stage of amorphous-nanocrystalline transformation. *J. Magn. Magn. Mater.*, accepted for publication (see also D.8.)

J.15. F. Mazaleyrat*, L.K. Varga: Ferromagnetic nanocomposites. *J. Magn. Magn. Mater.*, accepted for publication

J.16. J. Olszewski*, L.K. Varga, J. Zbroszczyk*, W.H. Ciurzyńska*, M. Hasiak*, A. Błachowicz*: Magnetic behaviour of the amorphous and nanocrystalline $Fe_{92-x}Zr_7Cu_1B_x$ (x = 2 or 6) alloys. *J. Magn. Magn. Mater.*, accepted for publication)

J.17. B. Varga, A. Lovas, F. Ye*, X.J. Gu*, K. Lu*: Pressure dependence of nanocrystallization in amorphous $Fe_{86}B_{14}$ and $Fe_{85}Cr_1B_{14}$ alloys. *Mater. Sci. Eng. A*, accepted for publication

J.18. L.K. Varga, F. Mazaleyrat*, J.Kováč*, F. Alves*, A. Kákay: Soft magnetic properties of nanocrytalline $Fe_{100-x}Si_x$ ($15 < x < 34$) alloys obtained by rapid quenching. *J. Magn. Magn. Mater.*, accepted for publication

J.19. L.K. Varga, F. Mazaleyrat*, J. Kováč*, F. Alves*, A. Kákay: Magnetic properties of rapidly quenched $Fe_{100-x}Si_x$ ($15<x<34$) alloys. *Mater. Sci. Eng. A*, accepted for publication

J.20. L.K. Varga, L. Novák*, F. Mazaleyrat*: Effective magnetic anisotropy and and internal demagnetization investigations in soft magnetic nanocrystalline alloys. *J. Magn. Magn. Mater.*, accepted for publication

Conference proceedings

J.21. B. Varga: On the rate of $\alpha \leftrightarrow \beta$ transformation in Fe-rich Fe-Ni alloys. In: *Proc. of Scientific Conf. of the Fac. of Electrical Engineering and Informatics*, Eds.: B. Zagyi, M. Kovaliková, J. Ziman, Technical University of Kosice, Slovakia, 1999, pp. 157-160.

J.22. B. Varga, É. Zsoldos*, G. Gerencsér*, A. Lovas: Study of phase transformation in $Fe_{100-x}Ni_x$rapidly quenched alloys using thermomagnetic measurements. In: *Proc. 16th Int. Coll. on Advanced Manufacturing Technologies in Vehicle Industry, Balatonfüred, 1999*, Techn. Univ. of Budapest, pp. 49-54.

Book

J.23. G. Konczos, I. Bársony*, P. Deák*: *Introduction to Materials Science and Technology* (Textbook of the Technical University of Budapest for Ph.D. students in physics, 1998).

Others

J.24. L.K. Varga, F.I. Tóth, T. Kemény, P. Bánki: Method for the preparation of nanocrystalline magnetic powder for non-destructive crack testing. *Hungarian Patent* No. (1999)

K. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

L. Rosta, L. Almásy, M. Avdeev, S. Borbély, L. Cser, T. Grósz, E. Rétfalvi, L. Riecsánszky, Gy. Török

Our Institute is one of the three associates of the Budapest Neutron Centre operating and using the 10 MW Budapest Research Rector (BRR) on the KFKI site. This modern neutron source is open for the domestic and international user community and serves various tasks, such as basic and applied research in physics, chemistry, biology, materials science, as well as commercial utilisation and education. For neutron beam measurements different types of horizontal channels are available: seven thermal and two fast neutron channels; a tangential beam tube serves for the neutron guide system. The Neutron Spectroscopy Department on one hand operates several experimental stations located on the above beam-lines, on the other hand provides services for external users to perform experiments and exploit the obtained results. In 1999 nearly 50 experiments were completed by the local staff and in collaboration with national or foreign users coming from university, industrial or other research laboratories.

We operate at BRR a pine-hole collimation type small angle scattering (SANS) instrument and a triple axis spectrometer (TAS) both installed on neutron guides. The installation of another TAS instrument is under way on a thermal neutron beam. Our activity related to neutron scattering is based essentially on experiments performed on the above spectrometers, some special studies, however, were performed at other neutron source facilities e.g. at Saclay (France) where we shared the construction of the Spin-Echo spectrometer (MESS), some experiments were performed at HMI Berlin and FZ Jülich.

The activity of our team is focused on three major topics in condensed matter research, namely the investigation of structure and dynamics of *liquids* (e.g. various solutions, anisotropic fluids, biological based liquids), *soft materials* (gels, polymers, surfactants etc.) as well as materials properties of *solids* (metals, alloys, composites etc.). A few examples will be shortly described below.

Liquids. — *Binary liquid mixtures of methyl-substituted pyridines* with heavy water were studied by small- and wide-angle neutron scattering. These systems exhibit a closed loop phase diagram in concentration-temperature coordinates, the size of the loop depends on the position of the methyl group attached to the pyridine molecule. Measurements performed far below the lower critical solution temperature indicated that even in the macroscopically homogeneous phase the solution is microscopically not homogeneous. Further analysis of the data are in progress, aiming to resolve the inhomogeneous structure, described by one parameter - the correlation length, into atomic scale models, where existence of pairs of methyl-pyridine molecules is expected to be shown. The derived structure of the series of methyl-substituted pyridines in water can be compared with recently performed quantum-chemical calculations.

The *aggregation of Brij-35 ($C_{12}EO_{23}$) non-ionic surfactant in aqueous solutions* has been studied by small-angle neutron scattering. The aggregates were described as being polydisperse spheres with tethered polymer chains to their surface. The least-squares fit of the above model provided a detailed concentration and temperature dependence of the microstructural evolution of micelles.

Sodium and magnesium dodecyl sulfate mixed micelle systems. Significant difference in the behaviour of the mixed systems of surfactants in comparison with their individual solutions explains the great interest to these systems and their wide use in various areas of industry, household and other fields. Small-angle neutron scattering (SANS) is a powerful technique to study the structural features of the micellar systems, in particular in mixed solutions. The change of the parameters of micelles as a function of the relative concentration of the surfactants was followed at different values of the total concentration with the aim to determine the role of the counterion nature in the mixed micelle formation. This information is of interest for the modern molecular theory of mixed micelles.

Soft materials. — During the last year versatile activity was in progress in this field. New type of *ferrogels* was synthesized on the base of chemically cross-linked PVA with attached mono-domain magnetite particles. The dynamical properties of this system were studied by neutron spin- echo technique. Two kind of internal motion was observed. A damped soft oscillating motion with amplitude about 1 nm and the fast fluctuation of magnetisation inside the magnetite particles (Neel's relaxation) with characteristic time of 6.1 ns were also registered. The structure of so-called "intelligent" *hydrogels* with immense swelling degree (10^3) was studied by the use of small - angle neutron scattering. It was shown that the allyldextran junctions form a superstructure with quasi-period of about 130 nm. Aluminium silicate *aerogels* possess with strong piezoelectric properties making this materials potentially useful for various applications. Small-angle neutron scattering study revealed fractal structure of this system dominated by silica network. A correlation between the fractal dimensions and the degree of piezoelectric effect is observed. Long-time structural relaxation was observed in *poly(vinyl chloride)* below the glass transition temperature. The annealing of a slightly plasticized bulk polymer for a long time (about 150 days) at temperature T = 45^{o}C induces the significant growth of spatial correlation of chain segments. The local molecular redistribution tends to form compact domains with radius of 8 nm. Segmental dynamics in *poly(ethylene oxide) grafted to fullerene* was studied by the use of neutron spin echo technique. The segmental dynamics of the polymer strongly influenced the fullerene-polymer interaction because the hydrophilic part of the polymer chain shells around the hydrophobic fullerene. This effect reveals itself in the change of the exponent of the intermediate correlation function which, following the Zimm - model gives the value for the exponent varying between 0.4 - 06, depending on the temperature.

Solids. — Nuclear radiation induces important changes in the microstructure of metallic components of nuclear power plant and research reactors, influencing their mechanical properties. The investigation of this problem has primary interest for the safety and lifetime of such nuclear installations. For the characterization of this kind of nanostructures, small-angle neutron scattering technique is a very useful tool. We have carried out experiments on samples of irradiated reactor vessel material of VVER-440 type reactors. In our measurements irradiated as well as non-irradiated samples were compared and magnetic field was applied for viewing the magnetic structure effects of the materials. The data were analyzed by the inverse Fourier transformation method. A clear modification of the structure due to irradiation was obtained.

Nanoparticle-containing materials were investigated by SANS. At finemet (FeCuNbSiB) alloys using the magnetic field the magnetic and nuclear particle size distributions were measured. Samples containing different Si:B ratio contains different

nanoparticles (Fe or FeSi) . These types of materials can be very important for high frequency technology.

Instrumentation development. — In order to maintain a high level experimental research capacity at modest financial frames, we devote special efforts to enhance neutron beam intensity and develop various neutron scattering instrument components. The major current development at BRR (a joint programme with the Atomic Energy Research Institute) is the installation of a cold moderator for expanding our condensed matter research possibilities for the highly demanded *cold neutron* region. This liquid hydrogen cold neutron source has been assembled now on the reactor site and ready for final tests and installation in the reactor. For the improved transportation of the neutron beams the whole neutron guide system will be modernised. The installation of optimised supermirrors guides is under way.

On the spectrometer development side several projects are running. The application of area detectors in TAS technique and tests of a time of flight monochromator diffractometer are parts of one of our EU projects. Various beam forming components are also under development. Polarising monochromators and a new generation of multidisc type velocity selectors are being constructed.

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Grants

EU ERB-CT96-0057	Perfect crystal neutron optics (L. Rosta, 1997-2000)
EU ERB-CT98-0098	Cold neutron optimisation (L. Rosta, 1998-2001)
EU ERB PL96-9007	Neutron Round Table (L. Rosta, 1998-2001)
IAEA B5-HUN/8879	Condensed matter research (L.Cser, 1996-99)
OMFB 0478/97	High speed velocity selector development (L. Rosta, 1997-1999)
OMFB EO 097/97	Perfect crystal neutron optics (L. Rosta, 1997-2000)
OMFB EU-97-B4-98	Cold neutron optimisation (L. Rosta, 1998-2001)
OMFB EI-65/98	Neutron beam sources (L. Rosta, 1998-2000)
OTKA T 025747	Structure of polymer solutions (S. Borbély, 1998-2001)
OTKA T 22486	Investigation of sintering processes (T.Grósz, 1997-2000)

Publications

Articles

K.1. Q. Ye*, S. Borbély, G. Horvai*: Microstructure of ion-selective plasticized PVC membranes studied by small-angle neutron scattering. *Anal. Chem.* **71**, 4313-4320 (1999)

K.2. A. Jákli, L. Almásy, S. Borbély, L. Rosta: Memory of silica aggregates dispersed in smectic liquid crystals: Effect of the interface properties. *Eur. Phys. J.* **B 10**, 509-513 (1999) (see also G.11.)

K.3. V.T. Lebedev*, G.A. Evmenko*, V.L. Alexeev*, D.N. Orlova*, Gy. Török, L. Cser, V.V. Klyubin*, A.A. Polyakov*, V.P. Budtov*, P.N. Moskalev*, A.I. Sibilev*, M.A. Sibileva*: Structure of Complexes of poly-N-vynilpyrrolidine with Samarium Diphtalocyanides in Aequeous Solutions. *Polymer Science* **A 41**, 777-783 (1999)

K.4. V.T. Lebedev*, Gy. Török, L. Cser, A.L. Buyanov*, L.G. Revelskaya*, A.I. Sibilev*, D.N.Orlova*: Polarized Neutron Study of Magnetic Ordering in Ferrogel. *Kollidn. Zh*. **61**, 1-6, (1999)

K.5. V.T. Lebedev*, Gy. Török: Analyse of Quasielastic Neutron Scattering in Solid state Using Filters Periodic in Space, *J. Techn. Letters* **25**, 77 (1999)

K.6. J. Šaroun*, P. Strunz*, S. Borbély, J. Ilavský*, B. Kolman*: Evaluation of high-resolution SANS measurements in multiple scattering regime. *Mat. Sci. Forum* **312-324**, 270-275 (1999)

K.7. Gy. Török, V.T. Lebedev*, L. Cser, A.L. Buyanov*, L.G. Revelskaya*: Neutron scattering study of polymer membranes based on interpenetrating network. *Mat. Sci. Forum* **312-324**, 470-474 (1999)

K.8. V.T. Lebedev*, Gy. Török, L. Cser, A.L. Buyanov*, L.G. Revelskaya*, D.N. Orlova*, A.I. Sibilev*: Magnetic Particle Structure Ordering in Ferrogel Under Applied Magnetic Field. *Mat. Sci. Forum* **312-324**, 773-778 (1999)

K.9. V.T. Lebedev*, Gy. Török, G.A. Evmenenko*, I.V. Golosovsky*, Gy. Káli*, L. Cser, D.N. Orlova*, A.I. Sibilev*, V.P. Budtov*: Influence of cyclic thermal treatment near the first order phase transition on the supramolecular structure of C_{60}. *Mat. Sci. Forum* **312-324**, 860-865 (1999)

K.10. V.T. Lebedev*, G.A. Evmenenko*, V.L. Alexeev*, D.N. Orlova*, Gy.Török, L. Cser, V.N. Zgonnik*, L.A. Vinogradova*, E.N. Melelevskaya*, E.E. Kever*, V.P. Budtov*, A.A. Polyakov* ,V.V .Klyubin*, A.I. Sibilev*, M.A. Sibileva*: Study of polivinilpyrrolidone-C_{60} complex in water solution by Neutron and light scattering and viscosimetry. *Mat. Sci. Forum* **312-324**, 1119-1124 (1999)

K.11. V.T. Lebedev*, Gy. Török, L. Cser, A.L. Buyanov*, L.G. Revelskaya*, D.N. Orlova*, A.I. Sibilev*: Magnetic phase ordering in ferrogels under applied field. *J. Magn. Magn. Mater.* **201**, 136-139 (1999)

K.12. V.T. Lebedev*, Gy. Török, Gy. Káli , L. Cser, D.N. Orlova*, A.I. Sibilev*: Dynamics of concentrated ferrofluid with labelled particles. *Journal of Magn. Magn. Mater.* **201**, 133-135 (1999)

K.13. V.T. Lebedev*, G.P. Gordeev*, A.I. Sibilev*, V.V. Klyubin*, Gy. Török, L. Cser, Gy. Káli, L.K. Varga: Neutron Spin Echo Study of Low-T_c Ferrofluid. *J. Magn. Magn. Mater.* **201**, 80-83 (1999) (See also J.8.)

K.14. S. Borbély, J.S. Pedersen*: Temperature induced aggregation in aqueous solutions of Pluronic F68 triblock copolymer containing small amount of o-xylene. *Physica* **B,** accepted for publication

K.15. S. Borbély, M. Heiderich*, D. Schwahn*, E. Seidl*: Resolution of the USANS diffractometer at the FRJ-2 research reactor in Jülich. *Physica* **B,** accepted for publication

K.16. S. Koizumi*, M. Annaka*, S. Borbély, D. Schwahn*: Fractal structures of a poly(N-isopropylacrylamide) gel studied by small-angle neutron scattering over a q-range from 10^{-5} to 0.1 $Å^{-1}$. *Physica* **B,** accepted for publication

K.17. T. Drucker*, A. Bóta*, S. Borbély: Layer formations of dipalmitoylphosphatidylcholine liposomes in the pretransition range. *Physica* **B,** accepted for publication

K.18. Sz. Vass*, J. Plestil*, P. Laggner*, S. Borbély, H. Pospisil*, T. Gilányi*, Simultaneous evaluation of SANS and SAXS patterns from caesium alkyl sulfate micelles. *Physica* **B,** accepted for publication

K.19. L. Almásy, L. Cser, G. Jancsó*: Neutron scattering investigations on aqueous solutions of 3-methylpyridine. *Physica* **B,** accepted for publication

K.20. E. Rétfalvi, Gy.Török, L.Rosta: Radiation damage study using small-angle neutron scattering. *Physica* **B,** accepted for publication

K.21. Gy. Török, V.T. Lebedev*, L. Cser, M. Zrinyi*: NSE-study of magnetic phase dynamics in poly(vynil alcohol) ferrogel. *Physica* **B,** accepted for publication

K.22. I.V. Golosovsky*, Gy. Török, E.I. Maltzev*, I. Mirabeau*: Neutron diffraction study of nanocrystalline alloys $Fe_{73.5}CuNb_3(Si,B)_{22.5}$. *Physica* **B,** accepted for publication

K.23. V.T. Lebedev*, Gy. Török, L. Cser, A.L. Buyanov*, L.G. Revelskaya*: Macrojunctions ordering in polyelectrolyte hydrogels. *Physica* **B,** accepted for publication

K.24. V.T. Lebedev*, Gy. Török, L. Cser: Long-time structural relaxation in poly(vinyl chloride) below glass transition. *Physica* **B,** accepted for publication

K.25. V.T. Lebedev*, Gy. Török, L. Cser, V.N. Zgonnik*, V.P. Budtov*, A. Brulet*, L.V. Vinogradova*, E.Yu. Melenevskaya*, D.N. Orlova*, A.I. Sibilev*: Segmental dynamics in stars of poly(ethylene oxide) chains grafted to fullerene. *Physica* **B,** accepted for publication

K.26. L. Cser, A. Gabriel*, M. Kocsis*, G. Messing*, L. Rosta, Gy. Török: Neutron measurements on the MK 200N-1 type 2-dimensional delay-line position sensitive detector with the new OTDCv1.11 time to digital converter. *Physica* **B,** accepted for publication

K.27. P. Konstantinov*, K. Krezhov*, E. Sváb, Gy. Mészáros, Gy. Török: Neutron powder diffraction refinement of the crystal structure of $La_4Ti_3O_{12}$. *Physica* **B,** accepted for publication (see also L.16.)

K.28. T. Hajdú*, L. Rosta: Optimisation of neutron velocity selector transmission by simulation. *Physica* **B,** accepted for publication

K.29. T. Grósz, V.A. Mityukhlyaev*, L. Rosta, A.P. Serebrov*, A.A. Zaharov*: Thermo-hydraulic test of the moderator cell of LH_2 cold neutron source at BNC. *Physica* **B,** accepted for publication

K.30. V. Garamus*, M. Avdeev, L. Rosta, I. Smirnova*, N. Smirnova*: SANS study of micelle formation in aqueous mixed solutions of sodium and magnesium dodecylsulfates with added salts. *Physica* **B,** accepted for publication

K.31. P. Harmat*, L. Bartha*, T. Grósz, L. Rosta: Sintered materials studied by SANS. *Physica* **B,** accepted for publication

K.32. K. Sinkó*, L. Cser, R. Mezei*, M. Avdeev, H. Peterlik*, G. Trimmel*, U. Schubert*, P. Fratzl*: Structure investigation of intelligent aerogels by small-angle neutron and X-ray scattering. *Physica* **B,** accepted for publication

Conference proceedings

K.33. L. Cser: Instrumentation for small-angle scattering. In: *Proc. Int. School and Symposium on Small Angle Neutron Scattering, Mátraháza, Hungary, October 8-11, 1998*, KFKI Report 1999-02/E, pp.1-11

K.34. S. Borbély, L. Barna*: SANS from Brij-35/SDS mixed solutions. In: *Proc. Int. School and Symposium on Small Angle Neutron Scattering, Mátraháza, Hungary, October 8-11, 1998*, KFKI Report 1999-02/E, pp.19-22

K.35. J. Plaček*, F. Szőcs*, I. Novák*, S. Borbély, R. Gilles*: Study of silica sorbents by SANS. In: *Proc. Int. School and Symposium on Small Angle Neutron Scattering, Mátraháza, Hungary, October 8-11, 1998*, KFKI Report 1999-02/E, pp.55-56

K.36. A. Timchenko*, M. Avdeev, I. Serdyuk*, O. Trubetskaya*, R. Oberthür*, H. Kihara, Study of humic acids by small-angle X-ray and neutron scattering. In: *Proc. Int. School and Symposium on Small Angle Neutron Scattering, Mátraháza, Hungary, October 8-11, 1998*, KFKI Report 1999-02/E, pp.83-86

K.37. P. Harmat*, O. Horacsek*, T. Grósz, L. Rosta: SANS investigation of sintered material: doped, sintered, deformed tungsten containing K bubbles. In: *Proc. Int. School and Symposium on Small Angle Neutron Scattering, Mátraháza, Hungary, October 8-11, 1998*, KFKI Report 1999-02/E, pp.95-100

K.38. L. Cser, L. Rosta, Gy. Kaszás*, Th. Krist*, F. Mezei: Investigation of Neutron Optical Multilayer Systems. In: *Proc. Conf. on „Materials Research Using Cold Neutrons at Pulsed Neutron Sources" Argonne, USA*, Eds.: P Thiyagarajan, F. Trouw, B. Marzec, C.-K. Loong, World Scientific Singapore, 1999, pp.152-157.

K 39. T. Grósz, P. Harmat*, O. Horacsek*, L Rosta: Small Angle Neutron Scattering Study of Oriented Dispersoids in Tungsten Wire. In: *Proc. Conf. on „Materials Research Using Cold Neutrons at Pulsed Neutron Sources" Argonne, USA*, Eds.: P. Thiyagarajan, F. Trouw, B. Marzec, C.-K. Loong, World Scientific Singapore, 1999, pp.169-173.

K.40. L. Rosta: Cold Neutron Source Development and Industrial Oriented Research at the Budapest Neutron Centre. In: *Proc. Conf. on „Materials Research Using Cold Neutrons at Pulsed Neutron Sources" Argonne, USA*, Eds.: P. Thiyagarajan, F. Trouw, B. Marzec, C.-K. Loong, World Scientific Singapore, 1999, pp.192-195.

K.41. L. Cser, Gy. Káli, L. Kőszegi, L. Rosta, Gy. Török: Neutron scattering study of hidden defects in aluminium based composite alloys. In: *Proc. Conf. on „Materials Research Using Cold Neutrons at Pulsed Neutron Sources" Argonne, USA*, Eds.: P. Thiyagarajan, F. Trouw, B. Marzec, C.-K. Loong, World Scientific Singapore, 1999, pp.158-159.

K.42. E.Rétfalvi, L.Rosta: SANS investigation of radiation induced damage of reactor pressure vessel steels, In: *Proc. of Int. Conf. on Experimental Nuclear Physics in Europe, June 21-26, 1999, Sevilla, Spain,* accepted for publication

K.43. V.T. Lebedev*, Gy. Török, L.Cser, V.N. Zgonnik*, L.V.Vinogradova*, E.Yu. Melenevskaya*, A. Brulet*, D.N. Orlova*, A.I. Sibilev*, V.P. Budtov*: Dynamics of star shaped macromolecules of polyethylene-oxide with C_{60} fullerene core. In: *Proc. Conf. Molecular Mobility and Order in Polymer Systems, St. Petersburg, June 7-10, 1999,* P063

K.44. V.T. Lebedev*, Gy. Török, L. Cser, A.L. Buyanov*, L.G. Revelskaya*, A. Brulet*, D.N. Orlova*, A.I. Sibilev*: Dynamics of hydrogels. In: Proc. Conf. *Molecular Mobility and Order in Polymer Systems, St. Petersburg, June 7-10, 1999,* P062

Book chapter

K.45. T. Jávorfi*, H. Amenitsch*, P. Laggner*, Z. Cseh*, L. Mustárdy*, S. Borbély, L. Rosta, G. Garab*: Nature of irreversible structural changes induced by intense light in the thylakoids. Small-angle X-ray and neutron scattering of magnetically aligned chloroplasts. In: *Photosynthesis: Mechanisms and effects*, Ed. G.Garab, Vol.1, Kluwer Academic Publishers, 1998, pp. 349-352

Others

K.46. S. Borbély, J.S. Pedersen*: Influence of o-xylene on the aggregation behavior of the Pluronic F68 triblock copolymer. In: *Annual Progress Report of the Condensed Matter Physics and Chemistry Department, RISŘ National Laboratory, Roskilde, Denmark*, Eds.: K. Bechgaard, K.N. Clausen, R. Feidenhans, I. Johannsen, 1999, p.112

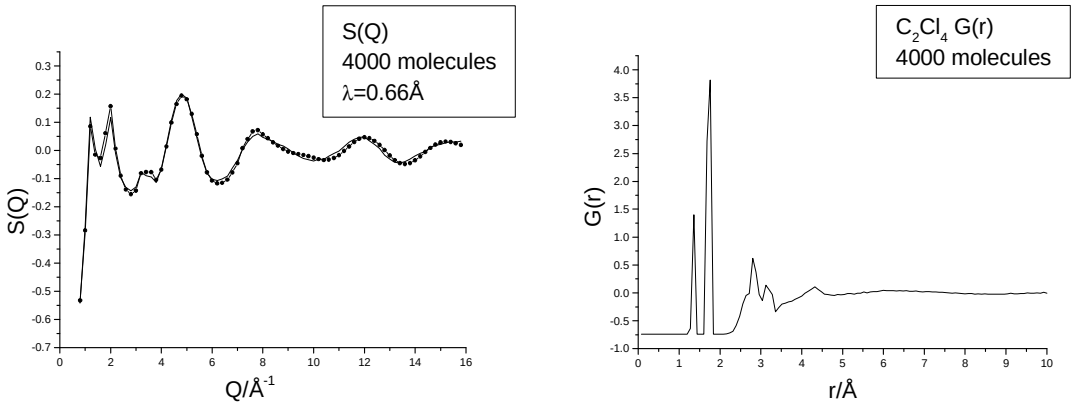
K.47. Gy. Kádár*, L. Rosta, Eds: *Lecture Notes on Neutron Scattering for the Introductory Course to ECNS'99.* Report KFKI-1999-04/E

L. NEUTRON SCATTERING

E. Sváb, P. Jóvári, L. Kőszegi, Gy. Mészáros, L. Pusztai, Z. Somogyvári

Molecular liquids. — Systematic studies on XCl_4 (X = C, Si, Ge, V, Ti and Sn) simple molecular liquids have been performed, consisting of neutron diffraction measurements using 1.057 Å neutrons on the powder diffractometer at the Budapest Research Reactor, and subsequent Reverse Monte Carlo (RMC) analyses. We have shown that the corner-to-face type orientational correlations, that had been thought to be dominant until recently in CCl_4, do not play significant role in either of the materials.

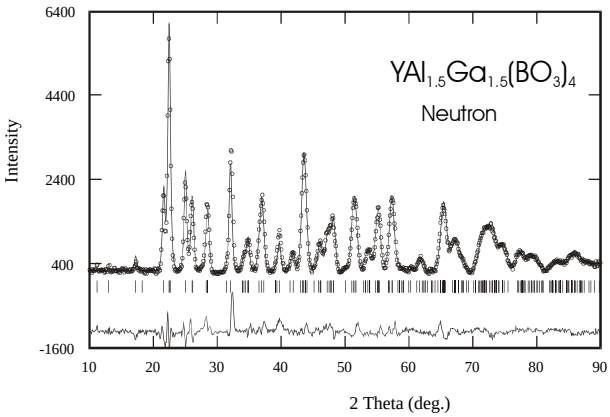
After an extension of the scattering vector range of the diffractometer up to 15 $Å^{-1}$, a series of measurements were carried out on simple molecular liquids such as CCl_4, C_2Cl_4, CBr_3D, CD_3I, CD_3OD, CD_3CN, Si_2Cl_6 and C_3OCl_6. By comparing different measurements made on CCl_4 and C_2Cl_4 we investigated the spatial information that can be safely extracted from experimental data by means of RMC simulation. It has been shown that the effect of possible experimental errors is much more controllable if large simulation boxes are used in RMC.



Experimental (dots) and fitted (solid line) structure factors for C_2Cl_4 and the total pair correlation function G(r), obtained by RMC

The structures of the three (liquid, high- and low-density amorphous) disordered forms of water have been modelled by the RMC method, based on existing (neutron and X-ray) diffraction data. The most important results of this new analyses are: (i) the H-bonding distance is larger (by about 0.1 Å) than suggested previously, in all the three phases; (ii) of the two amorphous ices, the low density form exhibits the larger H-bond disorder.

Oxides. — Crystal structure refinements were performed on various oxides with good optoelectronic or magnetoelectric properties. For $La_4Ti_3O_{12}$ the Rietveld refinement yielded considerably better reliability factors in the space group R-3 than those obtained in R-3m as suggested in the literature. The atomic coordinates and the thermal parameters were determined in this new space group.



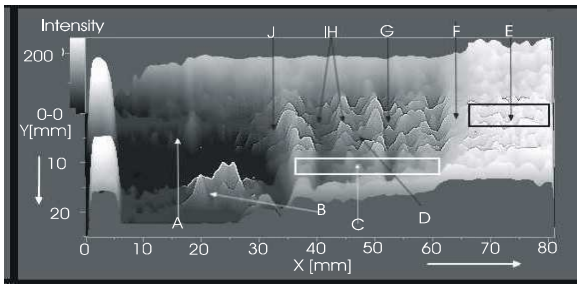
Neutron diffraction spectrum and Rietveld refinement of $YAl_{1.5}Ga_{1.5}(BO_3)_4$

The structure of $YAl_3(BO_3)_4$ and the effect of Ga-doping was analysed by combined neutron- and X-ray measurements. The refined crystallographic parameters were determined in space group R32. It was established that no lattice distortion is caused by Ga doping, while the lattice parameters increase by about 1 % .

Magnetite, Fe_3O_4 is a well known material which exhibits new properties when prepared on a nanoscale size of particles, e.g. the microwave absorption improves and the resonance frequency can be regulated by the grain size. The reason for this could be that the cationic distribution of Fe^{2+} and Fe^{3+} ions - which proved to be of high importance for the electric and magnetic properties of iron spinel - has changed in comparison with that of a microcrystalline material. Magnetic structure analyses by neutron diffraction have been undertaken on a series of nanocrystalline specimens.

Stress investigations were performed on Cu precipitates in $Fe_{95}Cu_5$ alloy. Temperature dependence of the (111) Bragg reflection of Cu was measured in the alloy and in a high purity Cu sample, respectively. While pure Cu simply follows the linear dependence found in the literature, the precipitated Cu grains in the alloy show peculiar behaviour. At the beginning the residual stress is tensile and changes its sign three times with rising temperature. These changes are reflected in the thermal expansion coefficient, as well.

Dynamic neutron radiography was applied to study the microstructure of oil containing reservoirs in a model experiment on Visingsö sandstone specimen. The characteristic features of the oil infiltration were visualized and analysed by image processing. Layered, laminated (I,H) petrophysical structures, oil infiltration zones (A,C), residual heavy water region (E), transient boundary layers (J,F) between them, non-absorbing thin friable segregations (B) and porosity (G) were disclosed.



Neutron radiography 3D image of an oil infiltrated specimen with the notations of the characteristic regions (see text)

Test measurements were performed on a recently purchased two-dimensional position sensitive neutron detector system (EMBL detector with OPEN Optoelectronics Ltd. electronics and software). The detailed investigations showed that the efficiency of this system is 2.6 % for 1.05 Å neutrons, instead of 37 % that could be expected from the specifications.

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OTKA T029433 Dynamic neutron-, gamma-, and x-ray radiography investigations and modelling of streaming processes (sub-contract E. Sváb, 1999-2002)

Publications

Articles

L.1. G. Tóth*, L. Pusztai, A. Baranyai*: Comment on: A new algorithm for Reverse Monte Carlo simulations [J. Chem. Phys. 109, 2634 (1998)]. *J. Chem. Phys.* **111,** 5620-5621 (1999).

L.2. L. Pusztai: On the partial pair correlation functions of liquid water. *Phys. Rev.* **B60**, 11851- 11854 (1999).

L.3. P. Jóvári: On the separation of inter- and intramolecular elastic neutron scattering intensity: the case of liquid CS_2. *Materials Science Forum* **321-324,** 492-495 (1999).

L.4. S.N. Ishmaev*, Z.V. Lisichkin*, A.V. Puchkov*, V.A. Semenov*, E. Sváb, G.F. Syrykh*: Neutron study of dynamic atomic correlations in amorphous isotopic Ni-B alloys. *Materials Science Forum* **321-324,** 502-506 (1999).

L.5. M.I. Mendelev*, S.N. Ishmaev*, F. Hajdu*, Gy. Mészáros, E. Sváb: Short-range order in Be-Zr metallic glass. *Materials Science Forum* **321-324,** 496-501 (1999).

L.6. K. Krezhov*, P. Konstantinov*, E. Sváb, Gy. Mészáros: Neutron diffraction investigation of cationic distribution in $Ni_xCo_{3-x}O_4$ spinels. *Materials Science Forum* **321-324,** 785-790 (1999).

L.7. M.Balaskó*, F. Kőrösi*, E. Sváb, I. Eördögh*: A novel type epithermic neutron radiography detecting and imaging system. *Nuclear Instr & Methods* **A424,** 263-269 (1999).

L.8. F. Kőrösi*, M. Balaskó*, E. Sváb: A distribution pattern of cadmium, gadolinium and samarium in Phaseolus vulgaris plants as assessed by dynamic neutron radiography. *Nuclear Instr & Methods* **A424,** 129-135 (1999).

L.9. M. Balaskó*, E. Sváb: Characterisation of segregation by dynamic neutron radiography. *Acta Phys. Polonica* **A96**, 7-18 (1999).

L.10. L. Pusztai: The structure of high- and low-density amorphous ice. *Phys. Rev. B,* accepted for publication.

L.11. P. Jóvári: Neutron diffraction and computer simulation study CS_2 and CSe_2. *Molec. Phys.,* accepted for publication.

L.12. L Pusztai, RL McGreevy*: MCGR: an inverse method for deriving the pair correlation function. *J. Neutron Res.,* accepted for publication.

L.13. L. Pusztai: How well do we know the structure of liquid water? *Physica B,* accepted for publication.

L.14. P. Jóvári, Gy. Mészáros, L. Pusztai, E. Sváb: Neutron diffraction studies on liquid CCl_4 and C_2Cl_4. *Physica B,* accepted for publication.

L.15. Gy. Mészáros,. E. Sváb, E. Beregi, A. Watterich, M. Tóth*: Rietveld refinement for yttrium aluminium borates from neutron- and X-ray diffraction. *Physica B,* accepted for publication. (See also R.12. and Q.15.)

L.16. P. Konstantinov*, K. Krezhov*, E. Sváb, Gy. Mészáros, Gy. Török: Neutron powder diffraction refinement of the crystal structure of $La_4Ti_3O_{12}$. *Physica B,* accepted for publication. (See also K.27.)

L.17. E. Sváb, M. Balaskó*, F. Kőrösi*: Dynamic neutron radiography in petrophysical application. *Physica B,* accepted for publication.

L.18. L. Kőszegi, Z. Somogyvári: Virtual thermal expansion coefficient of Cu precipitated in the $Fe_{95}Cu_5$ alloy. *Physica B,* accepted for publication.

Conference proceedings

L.19. M. Balaskó*, E. Sváb: Beam formation and filtering unit for thermal-, epithermal- and gamma radiation, In: *Proc. of 6th Word Conference on Neutron Radiography, Osaka, May 1999,* accepted for publication.

L.20. M. Balaskó*, E. Sváb, G. Endrőczi*, L. Komlódi*, I. Szikra*: Dynamic neutron radiography as a promoting method for modern NDT (thermovision, vibration diagnostics and acoustic emission) techniques. In: *Proc. of 6th Word Conference on Neutron Radiography, Osaka, May 1999,* accepted for publication.

L.21. M. Balaskó*, F. Kőrösi*, E. Sváb: Modelling of oil infiltration and distribution in sandstone applying dynamic neutron radiography. In: *Proc. of 6th Word Conference on Neutron Radiography, Osaka, May 1999,* accepted for publication.

L.22. F. Kőrösi*, M. Balaskó*, E. Sváb: Gadolinium transport and distribution in bean tissues studied by dynamic neutron radiography. In: *Proc. of 6th Word Conference on Neutron Radiography, Osaka, May 1999,* accepted for publication.

M. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, S. Varró, I. Bányász and K. Mocsár

Experiments with strong lasers on electrons in metals. — For studying laser-matter interactions in the ultra-intense (10^{18} W/cm^2) regime we have built a table top terawatt („T^3 ") chirped pulse amplification (CPA) neodymium phosphate glass laser system. Using this new system we have started experiments on both electron and photon emission processes of discrete (hν – structured) spectra predicted by our theoretical calculations.

We have performed experiments proving that a high energy x-ray field may be generated by shining laser light at grazing incidence on a gold target to create a surface plasma by applying, in addition, a strong static negative voltage to a metal plate parallel to the gold target at a small distance, such that the electrons are pushed back to the surface. With this arrangement powerful x-ray radiation of about 20 keV has been observed in the ns, ps and in the femtosecond range.

Theoretical study of interaction of strong laser fields and matter. —We have shown in the framework of quantum electrodynamics, that during a multiphoton-free-electron process, in which the Compton scattering occurs simultaneously with the elastic non-forward scattering of the other photons of the intense radiation field, the four momentum conservation allows the conversion of the ponderomotive energy into translational energy. The derived formulas may be used, for example, in the analysis of the above threshold ionization of atoms, in plasma physics and in astrophysics.

By considering a laser-induced oscillating double layer along the surface of a metal and its action on an electron of the metal, we have explained our recent experimental results on electron emission from gold cathodes irradiated by mid-infrared laser light (of wavelength up to 12 μm) in the MW/cm^2 regime. The theoretical formulae obtained reflect excellently back all the characteristics of the measured photoelectrons, namely the unexpectedly wide above threshold spectrum, the very high absolut current and the intensity dependence of the total current.

The above-mentioned laser induced double layer model gives also a satisfactory interpretation of our recent experimental resuls concerning the generation of strong x-ray pulses at metal surfaces in the presence of a static electric field.

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OTKA T16014	Experimental and theoretical investigation of new fundamental physical processes (laser-matter interactions) induced by laser beams of superintense, 10^{15}-10^{20} W/cm^2 laser systems (Gy. Farkas, 1995-1999)

TéT F-19/97 Interaction of laser radiation with solids (Gy. Farkas, 1997-1999)

Publications

Articles

M.1. F. Körmendi*, Gy. Farkas: Quantum electrodynamics of strong-field Compton scattering and its ponderomotive and drift energies. *Phys. Rev*. **A59**, 4172-4177 (1999)

M.2. I. Bányász, A. Beléndez*, I Pascual* and A. Fimia*: Comparison of nonlinear characteristics of phase holograms processed by various combinations of developers and bleaching agents. *Journal of Modern Optics* **46**, 591-605 (1999)

M.3. S. Varró, Gy. Farkas, F. Ehlotzky*: Generation of x-rays by irradiating metal surfaces with a powerful laser beam in the presence of a strong static electric field. *Opt. Commun.*, accepted for publication

M.4. S. Varró, Gy. Farkas, F. Ehlotzky*: High-order harmonic generation at metel surfaces in the presence of a strong static electric field. *Laser Physics*, accepted for publication

Others

M.5. S. Varró, Gy. Farkas: Diszkrét szerkezetű elektron-, ill. fényspektrumok fellépése szuperintenzív lézerterekben (Appearance of electron and light spectra of discrete structure in the presence of superintense laser fields, in Hungarian). In: *Lectures of the General Meeting, 1998,* Hungarian Academy of Sciences, Budapest, pp. 661-668 (1999)

M.6. Gy. Farkas, F. Körmendy*: Multi gigawattos laser-gyorsítók és terawatt/cm^2-es röntgenlaserek. In: *Lectures of the General Meeting 1998,* Hungarian Academy of Sciences, Budapest, pp. 669-673 (1999)

N. LASER PHYSICS

K. Rózsa, G. Bánó, L. Csillag, Z. Donkó, Á. Hoffmann, Z. Gy. Horváth, M. Jánossy, N. Kroó, K. Kutasi, Zs. Lenkefi, P. Mezei, K. Szőcs, Zs. Szentirmay

Gas laser studies — The cathaphoresis of zinc in the positive column of helium and neon discharges was studied experimentally. We measured the axial dependence of metal atom density along the positive column for different buffer gas pressures and discharge currents. The theoretical background of the zinc cathaphoresis was described by means of a model, which can also be applied for other metal-noble gas mixtures. Our results will be used in the design of the cathaphoretic confinement section of a heated laser tube, which will keep the metal vapour in the active region not allowing its diffusion toward the laser windows. We also carried out investigations of the mode structure of the segmented hollow cathode Au-II 690nm laser, giving information about the spectral properties of this kind of lasers. We observed single longitudinal mode operation for a wide range of discharge conditions. The time dependence of the laser output power was explained on the base of temperature and pressure changes after switching the discharge on.

Plasma experiments and modeling — We investigated the dynamical behavior of glow discharges using the technique of hybrid modeling. This approach combines the fluid description of ions and slow electrons with Monte Carlo simulation of fast electrons. The simulations were used to describe the self-generated oscillations developing in low current discharges. Another subject of our studies was the transient behavior of an argon discharge, which – due to the application of a high-voltage pulse – changes from the low current (Townsend discharge) to a high-current diffuse glow discharge. We also carried out spatially resolved emission spectroscopy investigations on argon glow discharges and nitrogen discharges applicable for policianide (CN_x) layer deposition. We developed a molecular dynamics simulation program to investigate the properties of strongly coupled electron – hole bilayers.

Electrolyte cathode atmospheric glow discharge (ELCAD). — Investigations have been performed on the electrolyte cathode glow discharge, which contained Pb metal. A significant increase was observed in the intensity of the Pb-I 405.8 nm atomic line, this occuring in the form of spikes. The frequency of the intensity spiking could be enhanced by increasing discharge current and Pb concentration of the electrolyte cathode.

Lookig at various energy schemes, it was found that there is a resonant energy coincidence between the upper level of the Pb-I 405.8 nm transition and the 4.4 eV excited state of the OH-radical. On the basis of this coincidence, the intensity increase can be attributed to energy transfer collisions of the second kind taking place between the Pb atoms and OH-radicals.

Determination of optical and surface morphological parameters on fullerene films. —A device was constructed for C_{60} sublimation at 450–500 °C in 10^{-4} Pa pressure. Thin films of 40–600 nm thickness were prepared at different substrate temperatures and evaporation rates. The complex dielectric function of samples was determined with an ATR reflectometer in the 400–900 nm wavelength range. Simultaneously, surface roughness parameters, as rms amplitude and correlation length, were determined with atomic force microscopy (AFM).

Drastic change of roughness structure was observed in function of substrate temperature which, on the other hand, strongly influenced the optical parameters of fullerene layers. The results are in correlation with our earlier observations made by gold layers evaporated on LiF substrates of different surface morphology.

Research on multidimensional lasers. — As a result of our research on multidimensional lasers, a point-source like laser emission, revealed by collapse of the emitted spectrum, has been observed from Rhodamine 6G dye droplets on optically mat surfaces. This shows that it is possible to achieve resonator-free laser operation in homogeneous laser materials without the presence of suspended, highly scattering micro-particles such as those used in laser paints. In our experiment a three-dimensional speckle pattern is created by the interference of coherent pumping light and its scattered distribution from a mat surface on which the Rhodamine droplet is placed. This temporally formed three-dimensional, statistical gain and/or refractive index modulation, i.e. speckle structure, will then result in laser operation in a manner similar to that produced in usual distributed feedback lasers. The study of resonator-free laser processes is important in order to understand the spontaneous laser processes possibly occuring in nature.

Laser application in biophysics. — In the field of biophysics the porphyrin synthesis of E. coli bacteria was stimulated by ALA-induction. The type of endogeneous porphyrins was determined using a high performance liquid chromatograph. MPIX and CPIII was found in the culturing medium and PPIX and MPIX inside the cells as major components. The spectral complexity of in vivo cells due to the endogeneous porphyrin mixture made it unable to draw conclusions about the location of the porphyrins inside the cells. This problem has been studied using site selective low temperature laser fluorescence spectroscopy and an approximation of the porphyrin environment has been made. The inhomogeneous distribution function (IDF) of endogeneous porphyrins of in vivo E. coli cells was determined. The gaussian decomposition of the IDF results in 3 components. The half width of the components indicates a liposome-like environment, based on comparison with porphyrin model solutions.

One step imaging ellipsometry. — In cooperation with a research group of ATKI- a new laboratory setup for speckle noise reduction has been constructed. Using a special, image capture synchronized modulation of the coherent laser light in the illuminating optical fibers, the contrast of speckle on the stored images was reduced to 1/100 of the original value, enabling the detection of the real, noise free ellipsometric data.

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Grants:

NATO SfP 971989 High beam quality UV lasers for Microelectronics (K. Rózsa, 1999-2004)
OMFB 01553/99 High beam quality UV lasers for Microelectronics (K. Rózsa, 1999-2004)
OTKA T-25941 Ultraviolet lasers in controllable-temperature hollow cathode discharge (K. Rózsa, 1998-2001)
OTKA T-25989 Numerical modeling of gas discharge plasmas (Z. Donkó, 1998-2001)
OTKA F-25503 Hollow cathode discharges and lasers in gold vapor (G. Bánó, 1998-2001)
OTKA T-017293 Multidimensional lasers (Z. Gy Horváth; 1996-1999)
OTKA T-029112 Excitation processes in electrolyte cathode atmospheric glow discharge (P. Mezei, 1999-2002)
OTKA T-020089 Optical parameters of fulleren films (Zs. Szentirmay, 1996-1999)
OTKA T-022074 Investigation of metal fulleren films with laser reflectometry (Á. Hoffmann, 1997-2000)

Publications

Articles

N.1. Z. Donkó: Modeling of low-current self-generated oscillations in a hollow cathode discharge. *J. Phys. D: Appl. Phys.* **32**, 1657-1664 (1999).

N.2. Z. Donkó, G. Bánó, L. Szalai, K. Kutasi, K. Rózsa, M. Pinheiro*, N. Pinhão*: Investigations on the effect of constriction in the cathode region of argon glow discharges. *J. Phys. D: Appl. Phys.* **32**, 2416-2425 (1999).

N.3. K. Szőcs, F. Gábor*, G. Csík*, J. Fidy*: Delta-Aminolaevulinic acid-induced porphyrin synthesis and photodynamic inactivation of Escherichia coli B. *J. Photochemistry and Photobiology* **B50**, 8-17 (1999).

N.4. M. Jánossy, P. Mezei: Excitation of the 210 nm Zn-II line in a He-Ne-Zn hollow cathode discharge. *Zeitschrift für Naturforschnung* ***A*****53**, 955-959 (1998).

N.5. G. Bánó, L. Szalai, K. Kutasi, P. Hartmann*, Z. Donkó, K. Rózsa, Á. Kiss, T. Adamowicz*: Operation characteristics of the Au-II 690 nm laser in a segmented hollow cathode discharge. *Appl. Phys.* **B**, accepted for publication.

N.6. P. Hartmann*, Z. Donkó, G. Bánó, L. Szalai, K. Rózsa: Effect of different elementary processes on the breakdown in low-pressure helium gas. *Plasma Sources Science and Technology*, accepted for publication.

N.7. Z. Donkó and B. Nyíri*: Molecular dynamics calculation of the thermal conductivity and shear viscosity of the classical one-component plasma. *Physics of Plasmas,* accepted for publication.

N.8. A.V. Phelps*, L.C. Pitchford*, C. Pedoussat* and Z. Donkó: Use of secondary electron yields determined from breakdown data in abnormal cathode-fall models for Ar. *Plasma Sources Science and Technology* (1999), accepted for publication.

N.9. L. Nemes*, M. Mohai*, Z.Donkó and I. Bertóti*: Detection of the CN radical in dc nitrogen plasma used for deposition of CNx layers. *Spectrochmica Acta Part* **A**, accepted for publication.

N.10. H.J. Kim*, J.H. Lee*, My. Kim*, T. Cserfalvi*, P. Mezei: Development of open-air type electrolute-as-cathode glow discharge-atomic emission spectrometry for determination of trace metals in water. *Spectrochimica Acta* **B**., accepted for publication.

Conference proceedings

N.11. J.H. Lee*, H.J. Kim*, S.Y. Yang*, T. Cserfalvi*, P. Mezei: Fundamental and analytical applications of electrolyte cathode atomic glow discharge (ELCAD) as a new source for on-line monitoring of metals in flowing waters. In: *Proc. of Colloquim Spectroscopicum Internationale XXXI. Sept. 5-10,1999, Ankara, Turkey*. Ed. Y. Ataman, Invited lectures IL-5.

N.12. Z. Donkó, G. Bánó, L. Szalai, K. Kutasi, K. Rózsa, M. Pinheiro*, N. Pinhão*: Investigations on discharge constriction in the cathode region of argon glow discharges. In: *Proc. of XXIII. International Conference on Phenomena in Ionized Gases (ICPIG)*, July 11-16, 1999, Warsaw, Poland, Contributed Papers Vol.3. pp.51-52 (1999).

N.13. P. Hartmann*, Z. Donkó, G. Bánó, K. Rózsa: Studies of electric breakdown in low-pressure helium gas. In: *Proc. of XXIII. International Conference on Phenomena in Ionized Gases (ICPIG), July 11-July 16*, 1999*, Warsaw, Poland* Contributed Papers Vol.4. pp.217-218 (1999).

N.14. M. Pinheiro*, N. Pinhão*, Z. Donkó: Electron Kinetics in Ne-Cu mixtures: Comparison between Boltzmann equation methods and Monte Carlo simulation. In: *Proc. of XXIII. International Conference on Phenomena in Ionized Gases (ICPIG), July 11-July 16, 1999, Warsaw, Poland,* Contributed Papers Vol.4. pp.171-172 (1999).

N.15. W. Kwasniewski*, Z. Donkó, L. Szalai, G. Bánó, K. Rózsa, and T. M. Adamowicz*: Evaluation of Au diffusion coefficient in He by 2-pulse excitation of a hollow cathode discharge. In: *Proc. of XXIII. International Conference on Phenomena in Ionized Gases (ICPIG), July 11-July 16, 1999, Warsaw, Poland,* Contributed Papers Vol.2. pp.83-84 (1999).

N.16. L. Szalai, G. Bánó, K. Kutasi, Z. Donkó and K. Rózsa: Optimization of hollow cathode discharges for pumping metal ion lasers. In: *Tenth International School on Quantum Electronics: Laser Physics and Applications, Bulgaria, Proc. of SPIE*, **3571**, 140-144 (1999).

Others

N.17. P. Mezei, T. Cserfalvi*, M. Jánossy: Atmoszférikus nyomású, elektrolitkatódos ködfénykisülés plazmafizikája. (Plasmaphysics of the electrolyte cathode atmospheric pressure glow discharge). In: *Fény-Anyag Kölcsönhatás, Kvantumoptika Tavaszi Iskola* (*Lecture on the Light-Matter Interactions, Quantumoptics Spring-School*, Pécs, Hungary, eds.: J. Bakos, Zs. Sörlei, S.Varró, pp. 88-95 (1999).

O. LASER APPLICATIONS

A. Czitrovszky, P. Apai, P. Jani, I. Kertész, Á. Kiss, M. Koós, S. Lakó, A. Nagy, I. Pócsik, J. Tóth, R. Szipőcs

Optical measuring techniques based on light scattering and interference. — Prototype Laser Doppler Anemometer equipment called *VELOSIZER* and software package was developed for the simultaneous measurement of the 2D velocity and size distribution of ultrafine (nanometer size) aerosol particles with high resolution, using photon counting technique and a high performance fast real time correlator. The system uses two single mode fiber illumination-detection setup making it particularly adaptable for measurement configurations hardly accessible otherwise.

Investigations of the elastic and inelastic properties of nanostructure of composite materials using a submicron resolution laser interferometric motion analysing *LIMAS* system were continued.

A quantum optical measurement system was developed for standardless measurement of the absolute value of the quantum efficiency of the photomultipliers and their noise at different temperatures. Several types of low noise, high gain photomultipliers were examined and measured. The developed new 16,000 channel multichannel analizer, provides also high time resolution measurements (coincidence, anticoincidence) with time/channel about 2ps.

The results of the optical particle counting and sizing measurements of the size distribution and concentration of the high temperature nuclear aerosols released from LWR fuel rods at 2000^{o}C in a large-scale nuclear accident simulation experiment in the frame of EU CODEX AIT program were analysed. The obtained data were compared with the results of integral aerosol collector and impactor measurements performed at the same time. The composition of the released particle was analized at different ingress periods.

The mechanical system of a differential particle mobility analyzer was designed, produced and combined.

Solid state laser development. — The development and application of Er:glass laser was continued. With a road of smaller diameter (3-4mm) and more efficient cooling the repetition rate grew to 3-5Hz. Two directions of the medical applications for the Er:glass laser are uniquely successful: heart surgery with high energy pulses and the combination with slit lamp for ophtalmology.

In the experiments for laser diode excitation different laser diodes (0.8μm and 0.97 μm, 10W) were used for Er^{3+}:Nd^{3+} and Yb^{3+} - Tm^{3+} - G^{3+} activated media. Effective laser radiation in the infrared (1,54μm and 1,06μm) and UV luminescence in the 204 – 312 nm region was observed.

Ultrafast laser technology. — In 1998, a new laboratory for ultrafast laser technique and laser spectroscopy was founded. Besides the scientific and technical expertise of the staff, the laboratory comprises a 10 W Ar-ion laser (Spectra-Physics), a tunable cw and femtosecond pulse Ti:sapphire laser (R&D Ultrafast Lasers Ltd.), a synchronously pumped, femtosecond pulse optical parametric oscillator (NT&C) and a high resolution double monochromator (CVI). The unique feature of the two femtosecond pulse systems is that they utilise chirped mirror (CM) technology for broadband feedback and intracavity dispersion control.

Optical thin film structures in femtosecond laser systems. — Dispersive dielectric mirrors were developed for different femtosecond laser systems such as: (a) novel, ion-beam-sputtered (IBS) multi-cavity Gires-Tournois mirrors (MCGTI) for mode-locked, mirror-dispersion-controlled, sub-100-fs tunable or low-pump-threshold, sub-15-fs Ti:sapphire lasers, (b) IBS chirped mirrors for broadly tunable cw and modelocked Ti:sapphire lasers and (c) ultrabroadband chirped mirrors for optical parametric amplifiers (OPA) in collaboration with R&D Lézer-Optika Bt., Hungary, and MLD Technologies, USA. The MCGTI mirrors exhibit reflectivities $R > 99.97\%$ and negative group delay dispersion of -50 ± 1 fs^2 over a bandwidth of 56 THz. The design of MCGTI mirrors was obtained by needle optimization. Dispersive properties of MCGTI mirrors originate from coupled resonances in multiple $\lambda/2$ cavities embedded in the layer structure. Alternatively, the design of our ultrabroadband chirped mirrors developed for the OPA system was obtained by our novel spatial frequency domain optimisation technique. The mirrors exhibit high reflectivity and a constant group delay dispersion over 210 THz and 140 THz, respectively, supporting sub-5-fs pulse generation in the visible with the OPA laser system built at the University of Tokyo. This OPA provides the shortest laser pulses ever obtained in the visible spectrum with a pulse duration of 4.7 fs.

Physics of mode-locked, femtosecond pulse Ti:sapphire lasers. — In collaboration with R&D Ultrafast Lasers Ltd., Hungary, a Gaussian approximation was developed for modelling the saturated gain in a highly pumped Ti:sapphire crystal. Using this model a soft-aperture Kerr-lens mode-locked laser was constructed delivering sub-10-fs pulses around 800 nm with an average output power of 1 W. The laser comprises IBS chirped mirrors and fused silica prism pairs for intracavity dispersion control. In collaboration with Philips Universität Marburg, Germany, phase properties of interference filters were discussed from the aspect of their use for phase-error-free wavelength separation of femtosecond laser pulses for ultrafast laser spectroscopy applications. It was found that high efficiency wavelength separation can be achieved by reflective intracavity filters built in femtosecond pulse laser or parametric oscillators.

Phase conjugation of femtosecond laser pulses in $BaTiO_3$. — Phase conjugation of spectrally broad femtosecond laser pulses was demonstrated by spectrally dispersing the pulses in a photorefractive $BaTiO_3$ crystal using our mode-locked Ti:S laser oscillator in cooperation with ICTP Trieste, Italy. Chirp of the phase conjugated femtosecond laser pulses was measured relative to the chirp of the incident pulse, and the group delay was found to be a smooth function of frequency.

Amorphous thin layers. — We have investigated the electronic levels related to π states of sp^2 hybridised, threefold co-ordinated carbon atoms of hydrogenated amorphous carbon (a-C:H) films by photoluminescence and direct current (dc) electrical conductivity (σ) measurements. These states constitute the top of the valence band and the bottom of the conduction band, and determine electrical and optical properties near the band edges. Surface enhanced Raman scattering (SERS) method was used to study the fine vibrational properties.

The temperature dependence of dc electrical conductivity of a-C:H layers does not exhibit Arrhenius type behaviour at and above room temperature. By increasing the temperature the actual activation energy (E_{act}), defined as the local gradient in a plot of the $\ln\sigma$ versus reciprocal temperature, increases continuously by a rate depending on the material properties. This sort of temperature dependence of dc conductivity is

expected when the distribution of tail states is very broad and the mobility edge is not sharp. In such a case the energy at which the dominant transport process takes place may change drastically with temperature. This argumentation gains strong support from our present results: that thermal annealing and higher deposition self bias decreases those potential barriers which localize the π electrons and results in much weaker dependence of E_{act} on temperature. After annealing, the actual activation energy decreases, and for samples deposited at -700V self bias E_{act} becomes nearly constant. The structural changes caused by thermal treatment and by deposition voltage were monitored by Raman scattering measurements.

We have observed, previously in the literature not reported, ultraviolet (UV) photoluminescence on soft a-C:H layers, which are prepared at low self-bias (-100 V) in plasma deposition process. Peak energy of two ultraviolet luminescence bands are much higher, than E_{04} optical gap of these amorphous carbon layers. The only mechanism, which can explain UV emission, is that both the excitation and emission takes place through localized states. If it is so the mobility edges are situated in deep of π state bands and observation of UV luminescence is an evidence for localization of nearly whole electronic levels related to π bonding states in soft a-C:H layers.

Surface enhanced Raman scattering (SERS) very effectively enhances the sensitivity of the Raman scattering by depositing rough silver island film onto the sample surface. Using silver colloid for preparing this film we have demonstrated, that this technique can successfully applied to study these a-C:H films as well. The improved resolution gives more details about the Raman spectra, the generally accepted two Gaussian interpretation can not hold any more.

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Grants

OTKA 020202	Development of fundamental experiments with squeezed light (A. Czitrovszky, 1996-1999)
OTKA T025707	Investigation on nano structures of composite metal-ceramic structures applying interferometric methods (P. Jani, 1998-1999)
OMFB 97-97-47-1539	Integrated optical sensor for the measurement of dynamic properties (P. Jani, 1997-1999)
OTKA T-026073	Electronic states, charge carrier localization and their interaction with the structure in amorphous carbon films (M. Koós, 1998-2000)

OTKA T-029578	Development of femtosecond pulse Ti:sapphire laser system utilizing chirped mirrors for dispersion control (R. Szipőcs
OTKA T-026073	Electronic states, charge carrier localization and their relation with the structure in amorphous carbon films. (M. Koós, 1998-2000).
OTKA T-025540	STM/AFM investigations of atomic and mesoscopic structures of amorphous carbon. (I. Pócsik, 1998-2000).
AKA 98-30 2,2	Solid State Carbon Structures: Structure on Atomic Scale, Experimental Investigations and Simulation (I. Pócsik, 1999-2000).
NATO SfP-973849	Carbon as Materials for Elecrochemical Storage of Energy (I. Pócsik, 1999-2003)

Publications

Articles

O.1. P. Jani, A. Czitrovszky, A. Nagy, R. Hummel*: Investigation of size distribution and concentration of aerosols released at CODEX AIT experiments. *Journal of Aerosol Science*, **30s**, 101-102 (1999).

O.2. A. Pintér Csordás*, L.L. Matus*, L. Maróti*, A. Czitrovszky, P. Jani: Aerosols released at high temperature oxidation of nuclear reactor core model. *Journal of Aerosol Science*, **30s**, 105-106 (1999).

O.3. M. B. Danailov*, K. Diomande*, P. Apai, R. Szipőcs: Phase-conjugation of broad-band laser pulses in $BaTiO_3$. *J. Mod. Optics*, **45**, 5-9 (1998).

O.4. M. Koós, I. Pócsik, S. Rebeja*, M. Iovu* and E. Colomeico*: Photoconductivity of a-C:H/p- Si Heterojunctions. *Balkan Physics Letters (BPL)* **6,** 262-267 (1998).

O.5. M. Koós, S.H. Moustafa, E. Szilágyi* and I. Pócsik: Non-Arrhenius Temperature Dependence of Direct-Current Conductivity in Amorphous Carbon (a-C:H) Above Room Temperature. *Diamond and Related Materials* **8,** 1919-1926 (1999).

O.6. P. Jani, A. Czitrovszky, L. Szótér*, J. Tajnafői*, B. Barna*, L. Molnár*: A laser interferometric motion analyser system and some of its applications. *Publ. of the Univ. of Miskolc, Hungary, Physics* **1**, 17-24 (1999)

O.6. P. Apai, S. Lakó, R. Szipőcs, M.B. Danailov*: Broad-band photorefractive phase conjugation in a dispersive scheme. *J. Laser Physics,* accepted for publication

O.7. R. Szipőcs, A. Euteneuer*, E. Finger*, M. Hofmann*, A. Kőházi-Kis*: Multi-color, mode-locked Ti:sapphire laser with zero pulse jitter. *J. Laser Physics,* accepted for publication

O.8. R. Szipőcs, A. Kőházi-Kis*, S. Lakó, P. Apai, A. P. Kovács*, G. DeBell*, L. Mott*, A. W. Louderback*, A.V. Tikhonravov*, M.K. Trubetskov*: Negative Dispersion Mirrors for Dispersion Control in Femtosecond Lasers: Chirped

Dielectric Mirrors and Multi-cavity Gires-Tournois Interferometers. *Appl. Phys. B*, accepted for publication

O.9. R. Szipőcs, A. Kőházi-Kis*, P. Apai, E. Finger*, A. Euteneuer*, M. Hofmann*: Spectral filtering of femtosecond laser pulses by interfernce filters. *Appl. Phys. B*, accepted for publication

O.10. M. Koós, E. Szilágyi* and I. Pócsik: UV Light Emission from Hydrogenated Amorphous Carbon (a-C:H) Layers. *Applied Physics Letters*, accepted for publication

O.11. A. Czitrovszky, A. Sergienko*, P. Jani, A. Nagy: Photometric measurements of quantum efficiency using quantum two-photon field. *J. Laser Physics*, accepted for publication

Conference proceedings

O.12. A. Czitrovszky, A. Nagy, P. Jani: Development of a new particle counter for simultaneous measurement of the size distribution, concentration and estimation of the shape-factor of liquid-borne particles. In: *18th Congress for Optics, San Francisco, 1999, SPIE* **3749,** 574-575 (1999).

O.13. P. Jani, A. Nagy, A. Czitrovszky: Nano-particle size distribution measurement in photon correlation experiments. In: *18th Congress for Optics, San Francisco, 1999, SPIE* **3749,** 458-459 (1999).

O.14. A. Czitrovszky, A. Sergienko*, P. Jani, A. Nagy: Absolute measurement of quantum efficiency of photon-counting photomultiplier using quantum two-photon field and a ratio between single- and double-electron peaks. In: *18th Congress for Optics, San Francisco, 1999, SPIE* **3749**, 422-424 (1999).

O.15. R. Szipőcs: Frequency domain synthesis of ultrabroadband chirped dielectric mirrors for sub-5-fs optical pulses. In: *Ultrafast Optics 99 conference, Monte Verita, Ascona, Switzerland, July 11-16, 1999*, pp. 130-133 (1999).

O.16. R. Szipőcs, G. DeBell*, A. V. Tikhonravov*, M. K. Trubetskov*: Multi-Cavity Thin-Film Gires-Tournois Interferometers For Broadband Dispersion Control in Femtosecond Lasers. In: *Ultrafast Optics 99 conference, Monte Verita, Ascona, Switzerland, July 11-16, 1999*, pp. 70-73 (1999).

O.17. A. Kőházi-Kis*, P. Apai, S. Lakó, R. Szipőcs: Modeling the saturated gain in Kerr-lens mode-locked Ti:sapphire lasers. In: *Ultrafast Optics 99 conference, Monte Verita, Ascona, Switzerland, July 11-16, 1999*, pp. 66-69 (1999)

O.18. R. Szipőcs, A. Kőházi-Kis*, P. Apai, E. Finger*, A. Euteneuer*, M. Hofmann*: Spectral filtering of femtosecond laser pulses by interference filters. In: *Ultrafast Optics 99 conference, Monte Verita, Ascona, Switzerland, July 11-16, 1999*, pp. 74-77 (1999)

O.19. I. Pócsik and M. Koós: Cooling rate dependence of T_g — caused by clustering. In: *Slow Dynamics in Complex Systems*, AIP Conference Proceedings **469**,

Woodbury, New York 1999, eds.: M. Tokuyama and I. Oppenheim, pp.: 557-558.

Books, bookchapters

O.20. M. Koós, I. Pócsik, J. Erostyák* and A. Buzádi*: Amorphous carbon luminescence: excitation and emission in a broad energy range. In: *Amorphous and Microcrystalline Semiconductors, Science and Technology,* Eds. S. Kugler and M. Stutzman, North-Holland, Amsterdam, 1998. pp.: 579-582.

O.21. I. Pócsik, M. Hundhausen*, M. Koós and L. Ley*: Origin of the D peak in the Raman spectrum of microcrystallline graphite. In: *Amorphous and Microcrystalline Semiconductors, Science and Technology,* Eds. S. Kugler and M. Stutzman, North-Holland, Amsterdam, 1998. pp.: 1083-1086.

O.22. S.H. Moustafa, M. Koós and I. Pócsik: DC electric properties of amorphous carbon with different bonding hybridization. In: *Amorphous and Microcrystalline Semiconductors, Science and Technology,* Eds. S. Kugler and M. Stutzman, North-Holland, Amsterdam, 1998. pp.: 1087-1091.

O.23. A. Czitrovszky, P. Jani, A. Nagy: Development of light scattering airborne particle counter and its application in the envoronmental monitoring. In: *Laser Diagnostics of the Atmosphere*, Ed. G. Denardo, M. Danailow, Trieste ICS, accepted for publication

Other

O.24. A. Czitrovszky, A. Nagy, P. Jani, A. Sergienko*: Kvantumoptikai mérési módszerek alkalmazása a fotometriában (Application of the quantum optical measurement methods in photometry, in Hungarian). In: *National school on light-matter interaction and quantum optics*, pp. 193-205, MTA Pécs 1999.

P. OPTICAL THIN FILMS

K. Ferencz

Optical thin film structures in femtosecond laser systems. — Continuing our research started in 1993, dispersive dielectric mirrors were developed for different femtosecond laser systems such as low-loss chirped mirrors for mode-locked Cr:LiSGaF, Cr:LiSAF lasers, broadly tunable cw and modelocked Ti:sapphire lasers, as well as IR KTP based parametric oscillators and high power femtosecond amplifiers. Special ultrabroadband chirped mirrors have been developed for pulse compression experiments at the University of Groningen, the Netherlands and at the Technical University of Vienna, Austria. The pulse duration of the compressed pulses is below 5 fs at both laboratories. Using the high power compressed pulses of the commonly developed Ti:sapphire amplifier system built at the TU Vienna, coherent X-ray emission was detected from a laser induced He plasma in the water window. The aim of the present development is generation of X-ray radiation having higher power, which makes it possible for practical applications such as X-ray microscopy and microlithography. Special X-ray filter sets was developed for these applications.

Other developments on optical coatings. — Low loss dielectric mirrors have been developed for hollow cathode copper and gold lasers. The mirrors have been successfully tested at the Department of Laser Physics. Our work on optical waveguides deposited on optical gratings are still in progress for optical sensors used for medical applications. We investigated the effect of surface relief grating on the morphology and waveguiding properties of the deposited dielectric layers. Transparent electrodes were developed for porous silicon light emitters.

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Publications

Article

P.1. G. Cerullo*, M. Nisoli*, S. Stagira*, S. De Silvestri*, G. Tempea*, F. Krausz*, K. Ferencz: Mirror-dispersion-controlled sub-10-fs optical parametric amplifier in the visible. *Optics Lett.* **24,** 1529-1531 (1999)

Conference proceeding

P.2. G. Cerullo*, M. Nisoli*, S. Stagira*, S. De Silvestri*, G. Tempea*, F. Krausz*, K. Ferencz: Generation of sub-10-fs pulses in the visible by a highly compact optical parametric amplifier. In: *1999 OSA Technical Digest (Novel Lasers and Devices - Basic Aspects), Munich, Germany*, Ed.: O. Svelto, 1999, pp. 66-68

Q. GROWTH AND CHARACTERIZATION OF OPTICAL CRYSTALS

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

Growth and study of nonlinear borate crystals. — Single crystals of β-BaB_2O_4 (BBO), LiB_3O_5 (LBO), $CsLiB_6O_{10}$ (CLBO), $Li_2B_4O_7$ (LTB), and $YAl_3(BO_3)_4$ (YAB) were grown by high temperature top-seeded solution growth (HTTSSG), Czohralski method and spontaneous nucleation, respectively. Chemical etching techniques have been developed and used for mapping and characterizing growth defects in these borates. The reliability of the different etching methods are demonstrated for the main crystallographic sections of the crystals. In the borates investigated, the directions of the polar axes can be assigned by the etching rate difference of the opposite sides. Growth imperfections such as twins, negative crystals, grain boundaries and dislocations were revealed. Twinning appeared by parallel lattice of the twin domains. Dislocations are predominantly inclusion induced. The formation of inclusions is the major limit in any improvement in crystal quality. In CLBO, at the sites of inclusions, the hydration process is increased and hasten the degradation of crystals. Removing surface defects by chemical etching helps to decrease surface degradation arising from crystal hydration at damages caused by mechanical operations as well.

Waveguides were formed in BBO single crystals by He^+ implantation on Y and Z cut samples. Refractive index profiles n_0 and n_e were reconstructed by the dark-line mode spectroscopy. The profiles show a step-like guiding region. Optical barriers with depth to $\Delta n_e = 0.04$ and $\Delta n_o = 0.1$ for Y-cut, and $\Delta n_e = 0.08$ and $\Delta n_o = 0.05$ for Z-cut sample are obtained. This is the first report on optical waveguide characterization in BBO.

The reaction path of the solid phase reaction of **YAB** was determined. In the starting $Y_2O_3:3Al_2O_3:4B_2O_3$ system, IR spectroscopy and X-ray diffraction data have shown that the expected $YAl_3(BO_3)_4$ formation (whose optimum temperature is at 1150 °C) was preceded and accompanied by the appearance of YBO_3 and $Al_4B_2O_9$ intermediate phases. At higher temperatures the $Al_{18}B_4O_{33}$ phase was also identified with both methods.

Growth and study of bismuth oxide based crystals. — Single crystals of pure and doped Bi_2TeO_5 were grown by the Czochralski technique. The first rare-earth doped crystal successfully grown was **Bi_2TeO_5:Er**. The basic absorption and luminescence spectroscopic properties of Er were determined in Bi_2TeO_5. From the temperature dependence and fine structure of the eight crystal field transitions observable in the transparent spectral range of the crystal, it was derived that Er occupies the three slightly different Bi sites.

OH-ions were first detected in Bi_2TeO_5 crystals. The O--H bonding is strongly oriented into the [100] crystallographic direction.

The most attractive feature of Bi_2TeO_5 is its photorefractive response that has been discovered in our institute. It was shown that the saturation diffraction efficiency (2%) in the former four-wave mixing experiments had been limited by the stability of the Ar-ion laser used. Applying a cw Nd:YAG laser (532 nm) for write, **the saturation diffraction efficiency was about 20%,** using the same geometrical arrangement as had been used in the former experiments (crystal orientation, polarization and crossing

angle of the write beams). This efficiency is highly competitive to the leading photorefractive materials.

Growth and study of stoichiometric lithium niobate crystals. — Single crystals of $LiNbO_3$ were grown with various compositions and dopants by the top-seeded flux and Czohralski techniques. The r(c) and r(22) electro-optic coefficients were determined as a function of the intrinsic defect concentration related to the deviation from the stoichiometry. The non monotonous dependence of the EO coefficients (and the corresponding dielectric permittivities) was attributed to the partial occupation of Li sites by Nb ions. Electromechanical contributions were also considered.

Novel luminescent centers have been observed in $LiNbO_3$:Cr,Mg crystals. A set of narrow emission lines were detected in the 770-850 nm region, in addition to the well known broad $^4T_2$ emission of the low field site Cr^{3+}, in the samples containing more than 4% Mg. All lines exhibit the same relaxation time and are strongly π polarized. Substitution of Mg by Zn produces the same lines, indicating that the Mg and Zn ions act as charge compensators in the defect structures and they are not directly incorporated in the novel center. Based on absorption, excitation, luminescence and fluorescence line-narrowing experiments, we associate the novel center with an exchanged coupled Cr center.

New spectroscopic data are presented on a stoichiometric $LiNbO_3$:Cr^{3+} sample produced by the top-seeded flux (HTTSSG) method. In this sample strong reduction of the “R-line” components was observed. The near infrared line that observable in the $LiNbO_3$:Cr^{3+} crystals (and in the $LiNbO_3$:Cr:Mg samples) was attributed to Cr^{3+}--Nb^{5+} pairs. All emission lines show an unprecedented small line width, which allows high resolution studies.

Growth and study of TeO_2 crystals. — The Czochralski grown single crystals of TeO_2 were irradiated by high energy electrons and low velocity heavy ions. New defects were identified after elevated temperature (above 125 °C) exposure by 2 MeV electrons. Amorphous track formation was observed after S, Zn, Mo, Kr, Te and Pb ion exposure that could be explained by the thermal spike model.

Analytical spectroscopic investigation of oxide crystals. — New method was developed and tested for determining the Er and Nd dopant in Bi_2TeO_5 crystals. The best solvent for the host crystal was concentrated HCl with a complex stabilizer, triammonium citrate. After optimizing the vaporization conditions, the detection limit of the graphite furnace atomic absorption technique was 4.9 mg/l and 131 mg/l for Er and Nd, respectively.

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Grants

OTKA T 014884 Growth and study of bismuth oxide based photorefractive materials (I. Földvári, 1995-99)

OTKA T 024091 Growth and study of nonlinear optical crystals transparent in the far UV region (K. Polgár, 1997-2000)

OTKA T 023737 Developing and applying spectroscopic methods for analyzing the dopants and trace elements in bismuth oxide based crystals (O. Szakács, 1997-99)

OTKA T 026647 Study of solid phase reactions for growth of nonlinear optical crystals (L. Pöppl (ELTE) and I. Földvári, 1998-2000)

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

HAS - CONACYT (Mexico) joint project: Growth, linear and nonlinear spectroscopy of new potential laser crystals (I. Földvári, 1998-2000)

HAS - Armenian Academy joint project: Growth and study of nonlinear optical crystals. (K. Polgár, 1996-2000)

COST Action P2. Application of nonlinear optical phenomena:

Project WG1/1. Materials and systems for optical data storage (I. Földvári, 1998-2001)

Project WG2/4. Nonlinear optics for quantum communication (K. Polgár, 1998-2001)

Publications:

Articles:

Q.1. I. Földvári, Á. Péter, O. Szakács, A. Munoz F*.: Improvement in quality and performance of photorefractive Bi_2TeO_5. *J. Cryst. Growth* **198-199,** 482-6 (1999).

Q.2. L. Bencs, O. Szakács, T. Kántor*: Determination of erbium and neodymium in bismuth tellurite optical crystals by graphite furnace atomic spectrometry techniques. *Spectrochim. Acta* **B 54**, 1193-1206 (1999).

Q.3. E. Beregi, E. Hartmann, L. Malicskó, J. Madarász*: Growth and morphology of Nd^{3+}, Er^{3+} and Cr^{3+} doped $YAl_3(BO_3)_4$ single crystals. *Crys. Res. Techn.* **34**, 641-45 (1999). (See also R.1.)

Q.4. T. Becze-Deák*, L. Bottyán*, G. Corradi, L. Korecz*, D. L. Nagy*, K. Polgár, S. Salem*, H. Spiering*: Electron trapping centres and cross sections in $LiNbO_3$ studied by ^{57}Co Mössbauer emission spectroscopy, *J. Phys.: Condens. Matter.* **11,** 6239-50 (1999). (See also R.6.).

Q.5. M. Aillerie*, K. Chah*, F. Abdi*, P. Bourson*, M.D. Fontana*, K. Polgár, G. Malovichko*: Influence of the non-stoichiometry on the electro-optic properties in pure $LiNbO_3$. *Ferroelectric*. **223**, 365-372 (1999).

Q.6. J.G. Marques*, A Kling*, J.C. Soares*, M.F. da Silva*, R. Vianden*, K. Polgár, E. Diéguez*, F. Agulló-López*: Structural defects in congruent and near stoichiometric $LiNbO_3$. *Rad. Eff. Def. in Sol.* **150**, 233-36 (1999).

Q.7. I. Földvári, R.S. Klein*, G.E. Kugel*, Á. Péter: Oxygen equilibrium and its detection in Bi_2TeO_5 crystals by Raman spectroscopy. *Rad. Eff. Def. in Sol.* **151**, 145-49 (1999).

Q.8. R. Capelletti*, I. Földvári, Á. Péter, L. Seravali*, The OH vibrational spectrum in Bi_2TeO_5 single crystals. *Rad. Eff. Def. in Sol.* **151**, 115-19 (1999).

Q.9. I. Földvári, A. Munoz F*., E. Camarillo*, Á. Péter, O. Szakács: Basic spectroscopic properties of Bi_2TeO_5:Er single crystals. *Rad. Eff. Def. Sol.* **149**, 55-59 (1999).

Q.10. L.A. Kappers*, O.R. Gilliam*, R.H. Bartram*, I. Földvári, A. Watterich: A study of optical and ESR radiation-induced absorptions in TeO_2 single crystals. *Rad. Eff. Def. Sol.* **150**, 161-66 (1999) (See also R.7.).

Q.11. R. Mouras*, P. Bourson*, M. Fontana*, M. Aillerie*, F. Lhommé*, K. Polgár: Influence of the MgO doping concentration on the width of the E(T01) Raman mode in congruent $LiNbO_3$ crystals. *Rad. Eff. Def. Sol.* **150**, 255-58 (1999).

Q.12. L. Grigorjeva*, D. Millers*, G. Corradi, K. Polgár, V. Pankratov*: Induced optical absorption and relaxation process in $LiNbO_3$. *Rad. Eff. Def. Sol.* **150**, 193-98 (1999). (See also R.10.).

Q.13. F. Lhommé*, P. Bourson*, K. Polgár, M. Aillerie*, M. Fontana*: Study of the luminescence spectra of $LiNbO_3:Cr^{3+},Mg^{2+}$; Effect of the concentration of Mg^{2+}. *Rad. Eff. Def. Sol.* **150**, 265-69 (1999).

Q.14. A. Skvortsov*, K. Polgár, L. Jastrabik*: Stark effect on f-f- spectra of $LiNbO_3:Er^{3+}$,Mg crystals. *Rad. Eff. Def. Sol.* **150**, 287-91 (1999).

Q.15. Gy. Mészáros,. E. Sváb, E. Beregi, A. Watterich, M. Tóth*: Rietveld refinement for yttrium aluminium borates from neutron- and X-ray diffraction. *Physica B,* accepted for publication (See also L.15. and R.12.).

Q.16. V. Pankratov*, L. Grigorjeva*, D. Millers*, G. Corradi, K. Polgár: Luminescence of ferroelectric crystals: $LiNbO_3$ and $KNbO_3$, *Ferroelectrics*, accepted for publication (See also R.13.).

Q.17. E. Beregi, A. Watterich, L. Kovács, J. Madarász*: Solid State Reactions in $Y_2O_3 : 3Al_2O_3 : 4B_2O_3$ System Studied by FTIR Spectroscopy and X-Ray Diffraction, *Vibrational Spectroscopy*, accepeted for publication (See also R.11.).

Q.18. Á. Péter, K. Polgár, E. Beregi: Revealing growth defects in non-linear borate single crystals by chemical etching. *J. Crystal Growth,* accepted for publication

Q.19. I. Földvári, K. Polgár, Á. Péter, E. Beregi, Zs. Szaller: Growth and study of nonlinear optical crystals at the Hungarian Academy of Sciences. *J. Telecom. Inform. Techn.,* accepted for publication

Q.20. I. Földvári, A. Munoz F*, E. Camarillo*, Á. Péter, R. Sosa F*: Basic optical absorption of Er in Bi_2TeO_5 single crystals. *Opt. Mater.*, accepted for publication

Q.21. A. Boudrioua*, P. Moretti*, J.C. Loulergue*, K. Polgár: Helium ion-implanted planar waveguide in Y-cut and Z-cut β-BBO (BaB_2O_4). *Opt. Mater.*, accepted for publication

Q.22. S.A. Basun*, G.M. Salley*, A.A. Kaplyanskii*, H.G. Gallagher*, K. Polgár: L. Lu*, U. Happek*: A novel luminescent center in $LiNbO_3$:Cr:Mg crystal. *J. Lumin*., accepted for publication

Q.23. G.M. Salley*, S.A. Basun*, A.A. Kaplyanskii*, R.S. Meltzer*, K. Polgár, U. Happek*: Chromium centers in stoichiometric $LiNbO_3$. *J. Lumin*., accepted for publication

Q.24. G. Szenes*, F. Pászti*, Á. Péter, A.I. Popov*, E. Balanzat*: Tracks induced in TeO_2 by heavy ions at low velocities. *Nucl. Instr. Meth. Phys. Res. B.*, accepted for publication

Conference proccedings

Q.25. L.A. Kappers*, O.R. Gilliam*, R.H. Bartram*, A. Watterich, I. Földvári: ESR of a radiation-induced defect in paratellurite. March Meeting of the American Physical Society, Atlanta, GA, March 1999. *Bull. Amer. Phys. Soc.* **44**, 369 (1999) (See also R.17.)

Q.26. L. Malicskó, A. Tóth*, E. Beregi: Microscopic studies of imperfections in selected YAB single crystals. In: *Proc. IV. Multinational Congress on Electron Microscopy*, Veszprém, Hungary, September, 1999. pp: 345-46. (see also R.16.).

Q.27. Z.E. Horváth*, B. Pécz*, Á. Péter, G. Szenes*: Amorphization of TeO_2 crystal by high energy ion iradiation. In: *Proc. IV. Multinational Congress on Electron Microscopy*, Veszprém, Hungary, September, 1999. pp: 323-24.

Q.28. I. Földvári, C. Denz*, Á. Péter, J. Petter*, F. Visinka*: Photorefractive performance of and image writing in bismuth tellurite. In: *Proc. Photorefractive Materials, Effect and Devices PR'99*, Lo-Skolen, Denmark, June 1999. Post deadline papers pp: 47-50.

Q.29. L. Kovács, E. Beregi, K. Polgár, Á. Péter: FTIR spectroscopy of borate crystals. *Proceedings of SPIE (International Conference on Solid State Crystals,* Zakopane, Poland*)* **3724**, 256-259 (1999). (see also R.14.).

Others

Q.30. T. Kántor*, L. Bencs, O. Szakács: Nehezen párolgó mintakomponensek in-situ elválasztása és meghatározása halogénezéssel kombinált grafitkemencés elektrotermikus párologtatás alkalmazásával (Separation and determination of heavily vaporized sample components by the application of graphite furnace electrothermal vaporization combined with halogenation, in Hungarian), *Proc.*

42nd Hungarian Conference on Spectrochemistry, Veszprém, June 28-30, 1999. pp. 1-5.

Q.31. L. Bencs, O. Szakács, T. Kántor*, G. Bozsai*: Optimalizációs eljárások bizmut-tellurit egykristályok adalékelemeinek dúsítására grafitkemencében atomabszorpciós meghatározás céljából,(Optimalization procedures for the preconcentration of dopant elements of bismuth tellurite single crystals in graphite furnace for atomic absorption spectrometry, in Hungarian), *Proc. 42nd Hungarian Conf. on Spectrochemistry*, Veszprém, June 28-30, 1999. pp. 6-11.

R. CHARACTERIZATION AND POINT DEFECT STUDIES OF OPTICAL CRYSTALS

A. Watterich, G. Corradi, E. Hartmann, L. Kovács, L. Malicskó, G. Mandula

Characterization of optical crystals. — The temperature dependence of the dc electrical conductivity of BaB_2O_4 crystals was measured from room temperature up to the melting point in vacuum by a two terminal technique using a new computer controlled arrangement which has been assembled recently. The electrical conductivity enabled to detect easily the alfa-beta transition of BaB_2O_4 crystals at in situ conditions. An abrupt change of the electrical conductivity showed that the transition of beta-BaB_2O_4 can already occur at 880 ^oC, which is a significantly lower value than the one reported in the literature (925 ^oC).

Microscopy of crystal imperfections. — The as-grown imperfections of $YAl_3(BO_3)_4$ single crystals grown from undoped and Nd^{3+} - doped flux ($K_2Mo_3O_{10}$ + B_2O_3) have been studied by optical and electron microscopic imaging and analytic methods. The as-grown composition and colour of these crystals have shown some locally correlating variation in different crystal regions. Some of these regions contained also small inclusions of other known molibdate phases originating from the flux. The real average composition of the $YAl_3(BO_3)_4$:Nd crystals can be described as $Nd_xY_{1-x-y}Al_{3+y}(BO_3)_4$ (B and O could not be analysed!).

The main conditions of the formation of the desirable (001) oriented and giant grained structure in semi- or superionic conductor polycrystalline Ag_2Se films were studied by optical and transmission electron microscopy. It has been established that this desirable structure can only be formed during heat treatments when at about 133 ^oC a slow polymorphic phase transition occurs simultaneously.

Point defects in $ZnWO_4$ and other oxide crystals. — After UV illumination at 77 K in $ZnWO_4$ single crystal the production of two new impurity related electron centres were detected by ESR: both defects are characterised as W^{5+}-type electron centres perturbed either by Sn^{4+} or Al^{3+} impurity ions substituting for Zn^{2+}, however, the position of the impurity ions must be different in the two defects.

In the isostructural $CdWO_4$ accelerated electrons at 273 K created two different ESR spectra. One of them can be greatly enhanced by reirradiating either by electron beam or UV (365 nm) light at 77 K. This latter spectrum is attributed to $V_O^{\cdot}$(A) and the other one to $V_O^{\cdot}$(B) centre known already in $ZnWO_4$. In these defects an oxygen vacancy trapped an electron (where A and B denotes the two possible, energetically different positions of the oxygen vacancies). This assignation is made on the basis of the similarity of the spin-Hamiltonian parameters of the corresponding centres in $ZnWO_4$. However, some differences are pointed out like formation temperature, different ratio of the two strongest W superhyperfine (SHF) interactions and additional SHF interactions in $CdWO_4$.

Infrared spectroscopy of hydroxyl ions in oxide crystals. — An infrared absorption band at about 3307 cm^{-1} was detected and attributed to the $0\rightarrow1$ stretching vibrational transition of hydroxyl ions (OH^-) in yttrium orthovanadate (YVO_4) single crystals grown by various methods. The isotopic replica (OD^-) in D_2O treated crystals was found at about 2455 cm^{-1} confirming the assignment above. The Morse-potential model was applied to determine the anharmonicity parameters of the hydroxyl

vibration. Polarization measurements showed that the OH^- dipoles lay in the plane perpendicular to the tetragonal axis. The temperature dependence of the band parameters was analysed using the model of weakly coupled phonons.

Asymmetric OH and OD stretch mode spectra have been observed in as-grown, congruent $LiTaO_3$, similarly to $LiNbO_3$. In vapour transport equilibrated stoichiometric $LiTaO_3$, however, the absorption bands become narrow and symmetrical. Although the phase transition temperatures for $LiTaO_3$ and $LiNbO_3$ are very different, the OH/OD spectra and the anharmonicities are very similar. This may suggest a behaviour of hydrogen in $LiTaO_3$ similar to $LiNbO_3$ e.g. in thermal fixing process of holograms.

Defect structure of $LiNbO_3$. — Electron-hole pair creation and charge transfer processes have been investigated in congruent and stoichiometric $LiNbO_3$ using several methods. Transient optical absorption and luminescence induced by laser or electron irradiation shows the majority of Nb^{4+} electron and O^- hole polarons recombining within 20 ns, the rest having longer decay times of the order of 1μs even at room temperatures. In congruent $LiNbO_3$, due to trapping at intrinsic defects, the long component tends to be longer and is non-radiative. For doped $LiNbO_3$ systems weaker dopant-specific luminescence bands and/or luminescence quenching have been observed. Using ^{57}Co Mössbauer emission spectroscopy the electron capture cross section of the dominating antisite niobium trap has been found to be smaller than that of Fe^{3+} traps, but still much larger than the cross section of Mg^{2+} traps.

Magneto-optic studies of Er doped $LiNbO_3$ crystals provided g-factor data for a large number of energy levels for various slightly different Er incorporation sites.

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Grants

OTKA T 022859 Determination of the structure of point defects by spectroscopic, conductivity and quantum chemical methods. (A. Watterich, 1997-2000)

OTKA T 023092 Characterization of multicomponent nonlinear optical crystals. (E. Hartmann, 1997-2000)

OTKA T 024092 Defect structure studies in $LiNbO_3$ crystals with various compositions and dopants (G. Corradi, 1997-2000)

OTKA T 026088 Fundamental processes of hologram fixing in photorefractive crystals. (L. Kovács, 1998-2001)

Portuguese-Hungarian Intergovernmental S&T Project, P 11/97: Growth, structural characterization and doping by ion implantation of stoichiometric $LiNbO_3$, lithium borates and bismuth tellurite (G. Corradi, 1998-1999)

Austrian-Hungarian Intergovernmental S&T Programme A-2/98: Thermal fixing of holographic gratings in stoichiometric $LiNbO_3$ crystals (L. Kovács, 1999-2000)

German-Hungarian Intergovernmental S&T Programme D-6/1998: Characterization of optoelectronic oxide crystals with advanced spectroscopic methods (G. Corradi, 1999-2001)

HAS-Polish Academy of Sciences joint project: Structure of real crystals (A. Watterich, 1999-2000)

Publications

Articles

R.1. E. Beregi, E. Hartmann, L. Malicskó, J. Madarász*: Growth and morphology of Nd^{3+}, Er^{3+} and Cr^{3+} doped $YAl_3(BO_3)_4$ single crystals. *Crystal Research and Technology* **34,** 641-645 (1999) (See also Q.3.).

R.2. G. Sáfrán*, L. Malicskó, O. Geszti*, G. Radnóczi* : The formation of (001) oriented Ag_2Se films on amorphous and polycrystalline substrates via polymorphic phase transition. *J. Crystal. Growth* **205,** 153-162 (1999).

R.3. A. Watterich, L. A. Kappers*, O. R. Gilliam*: Sn-related paramagnetic defects in UV-illuminated $ZnWO_4$ single crystals. *J. Phys.: Condensed Matter* **11**, 1333-1340 (1999).

R.4. L. Kovács, S. Erdei*, R.Capelletti*: OH^- vibrational band in YVO_4 crystals. *Solid State Communications* **111**, 95-99 (1999).

R.5. M. Wierschem*, C. Bäumer*, A. Jovanovic*, M. Wöhlecke*, S. Kapphan*, L. Kovács: Fundamental and overtone spectra of the OH and OD stretch mode in congruent and stoichiometric $LiTaO_3$. *Phys. Stat. Sol.* (b) **215**, R7 (1999).

R.6. T. Becze-Deák*, L. Bottyán*, G. Corradi, L. Korecz*, D. L. Nagy*, K. Polgár, S. Salem*, H. Spiering*: Electron trapping centres and cross sections in $LiNbO_3$ studied by ^{57}Co Mössbauer emission spectroscopy. *J. Phys.: Cond. Matter* **11,** 6239-6250 (1999) (See also Q.4.).

R.7. L. A. Kappers*, O. R. Gilliam*, R. H. Bartram*, I. Földvári, A. Watterich: A study of optical and ESR radiation-induced absorptions in TeO_2 single crystals. *Rad. Eff. Def. Solids* **150**, 161-166 (1999) (see also Q.10.).

R.8. P. Beneventi*, B. Briat*, R. Capelletti*, M. Gospodinov*, L. Kovács, E. Mazocchi*, A. Ruffini*: Electronic and vibrational levels of the photochromic Mn in sillenites. *Rad. Eff. Def. Solids* **150,** 243-247 (1999)

R.9. G. Corradi, L. Kovács and I. M. Zaritskii*: Optical absorption edge and some shallow donor levels in $LiNbO_3$ systems. *Rad. Eff. Def. Solids* **150,** 211-219 (1999).

R.10. L. Grigorjeva*, D. Millers*, G. Corradi, K. Polgár and V. Pankratov*: Induced optical absorption and relaxation process in $LiNbO_3$. *Rad. Eff. Def. Solids* **150,** 193-198 (1999) (See also Q.12.).

R.11. E. Beregi, A. Watterich, L. Kovács, J. Madarász*: Solid state reactions in Y_2O_3:$3Al_2O_3$:$4B_2O_3$ system studied by FTIR and X-ray diffraction. *Vibrational Spectroscopy,* accepted for publication (See also Q.17.).

R.12. Gy. Mészáros,. E. Sváb, E. Beregi, A. Watterich, M. Tóth*: Rietveld refinement for yttrium aluminium borates from neutron- and X-ray diffraction. *Physica B,* accepted for publication (See also L.15. and Q.15.).

R.13. V. Pankratov*, L. Grigorjeva*, D. Millers*, G. Corradi and K. Polgár: Luminescence of ferroelectric crystals: $LiNbO_3$ and $KNbO_3$. *Ferroelectrics,* accepted for publication (see also Q.16.).

Conference proceedings

R.14. L. Kovács, E. Beregi, K. Polgár, Á. Péter: FTIR spectroscopy of borate crystals. *Proceedings of SPIE (International Conference on Solid State Crystals, Zakopane, Poland)* **3724**, 256-259 (1999) (see also Q. 29.).

R.15. M. T. Borowiec*, H. Szymczak*, M. Zaleski*, P. Kaczor*, L. Adamowicz*, J. Strzeszewski*, A. Watterich, L. Kovács: Raman and IR spectroscopy investigations of double tungstates. *Proceedings of SPIE, (International Conference on Solid State Crystals, Zakopane, Poland)* **3724**, 288-291 (1999).

R.16. L. Malicskó, A. Tóth*, J. Beregi: Microscopic studies on imperfections in selected YAB single crystals. *Proc. IV. Multinational Congress on Electron Microscopy* (September 5-8, 1999, Veszprém, Hungary), 345-346 (1999) (see also Q.26.).

R.17. L. A. Kappers*, O. R. Gilliam*, R. H. Bartram*, A. Watterich, I. Földvári,: ESR of a radiation-induced defect in paratellurite. March Meeting of the American Physical Society, Atlanta, GA, March 1999. *Bull. Amer. Phys. Soc.* **44**, 369 (1999) (see also Q.25.).

R.18. G. Corradi: Nb^{4+} polaron and Ti^{3+} shallow donor Jahn-Teller centers in $LiNbO_3$ systems. In: *Proceedings of the NATO Advanced Research Workshop "Defects and surface induced effects in advanced perovskites", Jurmala, Latvia, 23-25 Aug., 1999*, invited paper, accepted for publication.

R.19. H. M. Yochum*, K. B. Ücer*, R. T. Williams*, L. Grigorjeva*, D. Millers* and G. Corradi: Subpicosecond laser spectroscopy of blue light-induced absorption in $KNbO_3$ and $LiNbO_3$. In: *Proceedings of the NATO Advanced Research Workshop "Defects and surface induced effects in advanced perovskites", Jurmala, Latvia, 23-25 Aug., 1999,* accepted for publication.

Others

R.20. L. Malicskó: Folyamat-indukálta kristályhibák oxidkristályokban.(Process-induced crystal defects in optical oxide crystals, in Hungarian). In: A Veszprémi Egyetem Speciális Kiadványa. Szerk.: Kovács K. (Special Transactions of the University of Veszprém. Ed. by K. Kovács.) Invited review paper, accepted for publication.

R.21. E. Hartmann: An introduction to crystal physics, *International Union of Crystallography*, http://www.iucr.acuk/iucr-top/comm/cteach/pamphlets/18/index.html (1998).

S. NONLINEAR AND QUANTUM OPTICS

P. Ádám, P. Domokos, J. Janszky, Zs. Kis, T. Kiss, M. Koniorczyk, Sz. Szabó, V. Szalay

Quantum state reconstruction. — We determined a class of time-dependent potentials that support the state reconstruction of one--dimensional wave packets. For this we extended the tomographic method for time--independent potentials to explicitely time--dependent situations. The existence of Wronskian pairs (regular and irregular wave functions) was assumed. We analyzed the consequences, and found a class of potentials for which the generalization is possible.

We analyzed our previously proposed scheme to reconstruct the quantum state of a one-mode travelling light field by cascaded optical homodyning. The local reconstruction of a quasiprobability function provided by the method can be applied to the approximate reconstruction of Glauber's R function by an analytic continuation. We found a simplified derivation of the sampling function occuring in the reconstruction by inverting the Radon transformation.

Cavity quantum electrodynamics and microlasers. — We developed the quantum theory of a single--mode thresholdless laser. We started from the basic Heisenberg-Langevin equations of motion for the field and atomic operators, and obtained an approximate analytical solution to these operator equations. We compared the predictions of this model for the intensity and power spectrum of the field to the results of a Monte—Carlo numerical simulation of the original Heisenberg—Langevin equations and found them in excellent agreement. We also compared these predictions to the ones of a rate equations model, which takes into account spontaneous emission. We showed that our model gives more reliable results in the bad cavity limit at high intensities. Based upon these results, we proposed a simple characterization of the thresholdless behavior. We applied our model to microsphere Nd-doped lasers at low temperatures, which are promising devices for a well--controlled thresholdless operation. We solved the basic differential equations of our analytical model by direct integration in the time domain (instead of the frequency one). The time-dependent solutions has been used to determine the higher-order correlations of the operator variables of the laser system. We found that the validity of the analytical model is limited in quantities corresponding to fourth-order correlations, such as for example the intensity noise.

Light propagation in quantized medium. — We have developed a simple model to describe the propagation of light in cold, quantized atomic medium. We have estimated the backaction of paraxially propagating light in a Bose-Einstein condensated dilute gas. We found that the two terms in the master equation describing the process in our model correspond to phase diffusion and depletion of the condensate. The estimation of the effect is in agreement with the phase-contrast imaging experiments.

Nonlocal quantum states and quantum teleportation. — We began to study nonlocal quantum phenomena in traveling-wave optical systems, that are important for confirming several fundamental questions of quantum mechanics, and may be elements of future's quantum communication networks. We have theoretically studied the quantum properties of light generated by a partially degenerate third order down-conversion process in detail. This process is capable of generating nonlocal quantum

states, in which one and two-photon states are entangled. We have shown, that with the aid of these states, arbitrary superpositions of a state with one photon state with a given polarization and a two-photon state with polarization orthogonal to that of the one-photon state, can be teleported. We have studied another teleportation scheme, that has connection with quantum state design, namely optical state truncation and teleportation with the method of projection synthesis. We have shown, that it is possible to truncate the Fock state expansion of an arbitrary one-mode optical state so that to leave components up to the n-photon states. For n=2, this is an experimentally realistic task. The process, nonlocal by nature, involves the teleportation of the resulting truncated state.

Trapped atoms.—We have examined the effects of the rarely appearing electronic transitions on the motion of a trapped ion in a Paul trap. We have worked out a master equation that includes the effects of laser-induced transitions and spontaneous emissions. We have shown how the electronic transitions give rise to important effects such as quantum decoherence and an asymmetric evolution of the system. If one is interested in studying the dynamics of the motional quantum state on long time scales, the effects of these quantum jumps become important.

Nuclear motions in molecules. — We have shown how contracted Hermite distributed approximating functions can be employed in solving vibrational eigenvalue problems. We have determined the best possible value of the barrier to linearity of water by high-quality *ab initio* quantum chemical methods. Small corrections due to one- and two-particle relativistic terms, core correlation effects, and the diagonal Born-Oppenheimer correction have been incorporated. We have developed the basic principles of the method of potential energy suface (PES) reconstruction. The reconstruction method gives an analytical approximation to a multidimensional PES from its sampled values which is eaqually accurate both on and off the sample points.

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Grants:

OTKA F 019232	Quantum optical processes in oscillator systems (Zs. Kis, 1996-1999)
OTKA T 023777	Effects of nonclassical states of light on atom optical phenomena (J. Janszky, 1997-2000)
OTKA F 023617	Phase squeezed and phase optimized quantum states of light (Sz. Szabó, 1997-2000)
OTKA T 025103	Vibrational potentional energy surfaces of molecules, the direct and the inverse spectroscopic problems (V. Szalay, 1998-2000)

Publications:

Articles

S.1. I. Protsenko*, P. Domokos, V. Levefvre*, J. Hare*, J. M. Raimond*, L. Davidovich*: Quantum theory of a thresholdless laser. *Phys. Rev.* **A 59**, 1667--1682 (1999).

S.2. U. Leonhardt*, T. Kiss, and P. Piwnicki*: Quantum backaction of optical observations on Bose-Einstein condensates. E*uro. Phys. J.* **D 7** 413-423 (1999).

S.3. U. Leonhardt*, T. Kiss, and P. J. Bardroff*: State reconstruction of wave packets moving in time--dependent potentials and the existence of Wronskian pairs. *J. Phys. A: Math. Gen*. **32**, 411-418 (1999).

S.4. M. Koniorczyk, J. Janszky and Z. Kis: Photon number teleportation, *Phys. Lett.* **A 256**, 334-338 (1999)

S.5. V. Szalay and S. C. Smith*: Application of contracted distributed approximating functions to solving vibrational eigenvalue problems. *J. Chem. Phys.* **110**, 72-79(1999).

S.6. G. Tarczay*, A. G. Császár*, W. Klopper*, V. Szalay, W. D. Allen*, and H. F. Schaefer III*: The barrier to linearity of water. *J. Chem. Phys.* **110**, 11971-11981(1999).

S.7. V. Szalay: Iterative and direct methods employing distributed approximating functionals for the reconstruction of a potential energy surface from its sampled values. *J. Chem. Phys*. **111**, 8804-8818 (1999).

S.8. C. Di Fidio*, S. Wallentowitz*, Z. Kis, W. Vogel*:Quauntum-jump effects in the motion of a Raman-driven trapped ion. *Phys. Rev.* **A 60**, R3393 (1999).

S.9. Z. Kis, T. Kiss, J. Janszky, P. Ádám, S. Wallentowitz* and W. Vogel*: Local sampling of phase-space distributions by cascaded optical homodyning. *Phys. Rev.* **A59**, R39-42 (1999)

S.10. Z. Kis, T. Kiss, J. Janszky, P. Ádám, S. Wallentowitz, and W. Vogel: Detection of non-classical oscillations in phase-space by cascaded optical homodyning. *Laser Physics*, accepted for publication.

S.11. P. Domokos, J. Hare*, V. Lefevre*, J. M. Raimond*, S. Haroche*, I. Protsenko*, L. Davidovich*: Quantum theory of microlasers in the close-to-threshold regime. *Laser Physics*, accepted for publication.

S.12. S. Szabó, P. Ádám, J. Janszky: Phase optimized states via coherent-state superpositions. *Laser Physics*, accepted for publication.

S.13. P. Ádám, A. Kárpáti, J. Janszky, E. Lugosi*: Relation between the input and output states of integrated optical systems. *Laser Physics*, accepted for publication.

Conference proceedings

S.13. M. Koniorczyk, J. Janszky, Z. Kis: Three photon states for quantum teleportation. In: *Proc. 6th Central-European Workshop on Quantum Optics, Olomouc, Acta Phys. Slov*. **49**, 707-712 (1999).

S.14. Z. Kis, T. Kiss, J. Janszky, P. Adam, S. Wallentowitz*, and W. Vogel*: Cascaded optical homodyne detection. In: Proc. 6*th Int. Conf. Squeezed States and Uncertainty Relations, NASA,* (invited paper) accepted for publication.

S.15. Z. Kis and J. Janszky:Generalized one-dimensional representation, In: Proc. 6*th Int. Conf. Squeezed States and Uncertainty Relations, NASA*, accepted for publication.

S.16. A. Karpati*, P. Adam, J. Janszky, M. Bertolotti*, C. Sibilia*: Sub-Poissonian light in integrated optical systems. In: Proc. *5th Int. Conf. Squeezed States and Uncertainty Relations, NASA*, accepted for publication

Others (technical digest, papers in Hungarian, etc.)

S.17. J. Janszky, M. Koniorczyk: Kvantumteleportáció (Quantum teleportation, in Hungarian). In: *Interaction of light with matter, quantum optics*, ed. J. Bakos et. al, Pécs, 1999 pp.1-10 (tutorial article).

S.18. P. Domokos: Kvantumelektrodinamika üregrezonátorban (Cavity quantum electrodynamics, in Hungarian). In: *Interaction of light with matter, quantum optics*, ed. J. Bakos et. al, Pécs, 1999 pp.160-180 (tutorial article).

EDUCATION

Graduate and postgraduate courses, 1999

- Advanced Solid State Physics (J. Sólyom, ELTE[5])
- Completely integrable many body systems (F. Woynarovich, JATE[6], Szeged)
- Statistical physics (F. Iglói, JATE)
- Thermodynamics and statistical physics (F. Iglói, JATE)
- Statistical Physics (P.Fazekas, BME[7])
- Magnetism I (P.Fazekas, BME)
- Magnetism II (P.Fazekas, BME)
- Optical Properties of Solid State (I. Tüttő, ELTE)
- Advanced Solid State Physics II. (I. Tüttő, ELTE)
- Solid state research I (I. Vincze, ELTE)
- Amorphous and crystalline materials (P. Deák*, S. Kugler* and T. Kemény, BME)
- Structure and Properties of Non-Equilibrium Alloys (T. Kemény, ELTE)
- Modern theory of nucleation (L. Gránásy, ELTE)
- Macromolecules (S. Pekker, ELTE)
- Spectroscopy and materials structure,(K. Kamarás, BME)
- Group theory in solid state research, (K. Kamarás, BME)
- Methods in materials science, (K. Kamarás BME)
- Synthesis of Liquid Crystals (K. Fodor-Csorba, ELTE)
- Physics of liquid crystals and polymers (Á. Buka and N. Éber, ELTE)
- Pattern formation in complex systems (Á. Buka, ELTE)
- Magnetic and magnetotransport properties of nanophase metals (I. Bakonyi, University of Bristol)
- Advanced material technology (G. Konczos, BME)
- NMR spectroscopy (K. Tompa, BME)
- Group theory in solid state research (G. Kriza, BME)
- Neutron Scattering (L. Cser, ELTE)
- Neutron Scattering in Condensed Matter (L. Rosta, BME)
- Neutron and X-ray Scattering for Structural and Dynamic Investigation of Condensed Matter (S. Borbély, BME)

[5] ELTE: Loránd Eötvös University, Budapest

[6] JATE: Attila József University, Szeged

[7] BME: Technical University of Budapest

- Optical methods in solid state physics (Zs. Szentirmay, ELTE)
- Physics of Non-Crystalline Matter and Glasses I. (M. Koós and I. Pócsik, JATE)
- Physics of Non-Crystalline Matter and Glasses II. (I. Pócsik and M. Koós, JATE)
- Crystal Physics of Optical Crystals (I. Földvári, Á. Péter, BME)
- Crystal Growth from the Melt (in: Crystalline and Amorphous Materials, K. Polgár, BME)
- Technical application of crystals. (E. Hartmann, BME)
- The growth and dissolution forms of crystals (E. Hartmann, BME)
- Theories of the crystal growth (L. Malicskó, BME)
- Microscopy in Materials Science (L. Malicskó, BME)
- Optical phenomena in solid state physics (L. Kovács, JPTE[8])
- Crystal optics and applications (L. Kovács, JPTE)
- Statistical quantum optics I. (J. Janszky, P. Ádám, ELTE)
- Statistical quantum optics II. (J. Janszky, P. Domokos, ELTE)
- Quantum mechanics (P.Ádám, JPTE)
- Quantum optics II. (J. Janszky, P. Ádám, P. Domokos, JATE)
- Fundamental quantum optical experiments (P. Ádám, T. Kiss, JPTE)
- Cavity quantum electrodynamics (P. Ádám, P. Domokos, JPTE)
- Modern experiments and paradoxes in quantum mechanics (M. Koniorczyk, P. Ádám, JPTE)
- Radiation theory (P. Ádám, JPTE)
- Atom traps (P. Ádám, T. Kiss, JPTE)

Laboratory practice and seminars

- Solid State Physics seminar (J. Sólyom, I. Tüttő, ELTE)
- Laboratory for solid state physics (I. Vincze, ELTE)
- Basic experimental physics (L. Gránásy, BME)
- Atomic and molecular physics laboratory, (K. Kamarás, ELTE)
- Basic experimental physics (A. Jákli, BME)
- Experiments on liquid crystals (Á. Buka, ELTE)
- NMR spectroscopy (K. Tompa, ELTE and BME)
- Solid state physics repetition (G. Kriza, BME)
- Superconductivity seminar (G. Kriza, BME)

[8] JPTE: Janus Pannonius University, Pécs

- Physical Chemistry Laboratory Practice (L. Péter, ELTE)
- Advanced solid state physics laboratory (I. Pethes and P. Matus, ELTE and BME)
- Neutron Scattering (BME, L. Rosta, Gy. Török)
- Experimental Methods in Neutron Physics (BME, L. Rosta)
- Medical application of lasers (Z. Gy. Horváth ; HIETE, Medical Laser Center)
- Laboratory practice and seminars on biophysics for medical students (K. Szőcs, SOTE)
- Seminars on laser optics (Zs. Szentirmay, ELTE)
- Laser optical laboratory (Zs. Szentirmay, ELTE)
- Quantum mechanics, (M. Koniorczyk, JPTE)

Diploma works

- B. Dóra (BME): Symmetry properties of the order parameter of unconventional spin density waves (Supervisor: A. Virosztek)
- R. Juhász (JATE): Critical behaviour of random quantum Ising model (Supervisor: F. Iglói)
- Z. Jurek (BME): X-ray diffraction studies of anisotropic solids (Supervisor: gy. Faigel)
- G. Gerencsér (BME): Thermomagnetic study of phase transformations in soft magnetic alloys (Supervisor: A. Lovas)
- P. Matus (BME): Study of ^{87}Rb NMR spin-lattice relaxation time in $Rb_{0.3}MoO_3$ (Supervisor: G. Kriza)
- T. Hajdu (BME): Optimisation of Neutron Transmission of Velocity Selectors (Supervisor: L. Rosta)
- L. Barna (BME): Aggregation in aqueous solutions of Brij-35 non-ionic detergent studied by small-angle neutron scattering (Supervisor: S. Borbély)
- Z. Somogyvári (BME): The microstructure of Fe(Cu5%) alloy studied by neutron diffraction (Supervisor: L. Kőszegi)
- K. Mocsár (BME): Generation of high intensity ultrashort laser pulses by a solid state laser system for experiments on light-matter interactions. (Supervisor: Gy. Farkas)
- K. Kutasi (JPTE): Babes-Bólyai University, Cluj, Romania: Hibryd model of a plane-parallel hollow cathode discharge. (Supervisor: Z. Donkó)
- M. Koniorczyk (ELTE): Nonlocality and quantum teleportation in multiple photon systems (Supervisor: J. Janszky)

Ph. D. students

E. Szabó (ELTE): Synthesis of achiral bent shaped molecules (Supervisor: K. Fodor-Csorba)

M. Bokor (ELTE): NMR relaxation in Fe and Zn ionic crystals (Supervisor: K. Tompa)

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

T. Marek (ELTE): NMR spectra in Fe and Zn ionic crystals (Supervisor: K. Tompa)

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

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

D. Goldschmidt (Host university: Otto von Guericke Universität): Interferometric studies of patterns in liquid crystals (Hungarian co-advisor: Á. Buka)

B. Varga (BME): Study of phase transformations in rapidly quenched micro- and nanocrystalline alloys by magnetic measurements (Supervisor: A. Lovas)

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

L. Almásy (ELTE): Investigation of metastable sytems by neutron scattering (Supervisor: L. Cser)

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

M. Avdeev (Dubna, IAEA): SANS Study of Soft Condensed Matter (Supervisor: L. Rosta)

P. Jóvári (ELTE): Neutron diffraction and computer simulation studies of molecular liquids (Supervisor: L. Pusztai)

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

G. Bánó (JATE): Cathode sputtered and heated Zn lasers in high voltage hollow cathode discharge (Supervisor: K. Rózsa)

K. Kutasi (JPTE): Modeling of glow discharges (Supervisor: Z. Donkó)

K. Szőcs (SOTE): Fluorescence imaging (Supervisor: Z. Gy. Horváth)

Said H.S. Moustafa (JATE): Amorphous carbon thin layers, structure and macroscopic physical properties (supervisor: M. Koós)

F. Lhommé (Host university: Université de Metz): Study of the intrinsic and extrinsic defects in lithium niobate doped with chrome. (Hungarian co-adviser: K. Polgár)

P. Domokos (ELTE): Cavity quantum electrodynamics (Supervisor: J. Janszky)

Z. Kis (JATE): Nonclassical vibrational states (Supervisor: J. Janszky)

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

Dissertations

S. Varró: Nonlinear processes of electrons in a strong laser field. (Doctor of the Hungarian Academy of Sciences)

T. Pusztai: Preparation and structural investigation of the photopolymer C_{60} (Ph.D., ELTE)

T. Börzsönyi: Instabilities in liquid crystals induced by mechanical and temperature field (Ph.D., ELTE)

Said H. S. Moustafa: Amorphous Carbon (a-C:H) - Atomic Bonding Structure, Electrical and Optical Properties (Ph.D. JATE)

S. Szabó: Low dimensional coherent state representations of the quantum states of light (Ph.D, ELTE)

T. Kiss: Methods to reconstruct the quantum states of light (Ph.D, ELTE)

AWARDS

- G. Faigel and M. Tegze, Széchenyi Prize of the Hungarian Republic
- G. Fáth, Bólyai Grant (1999-2002)
- K. Penc, Bólyai Grant (1999-2002)
- J. Sólyom, Széchenyi Professorship (1999-2002)
- P. Fazekas, Széchenyi Professorship (1998-2001)
- J. Kollár, Széchenyi Professorship (2000-2003)
- A. Virosztek, Széchenyi Professorship (1997-2000)
- D. Kaptás, Bólyai Grant (1999-2002)
- L. Gránásy, Award of the Research Institute for Solid State Physics and Optics (1999)
- L. Gránásy, Széchenyi Professorship (1999-2003)
- K. Kamarás, Széchenyi Professorship (1998-2002)
- G. Oszlányi, Bólyai Grant (1998-2001)
- T. Pusztai, Soros Grant (1998-1999)
- A. Jákli, Bólyai Grant (1998-1999)
- T. Tóth-Katona and T. Börzsönyi, Award for young Scientists of the Hungarian Academy of Sciences (1999)
- Á. Buka, Széchenyi Professorship (1998-2001)
- G. Kriza, Széchenyi Professorship (1999-2002)
- L. Pusztai, Bólyai Grant (1998-2000)
- Z. Donkó: Award of the Research Institute for Solid State Physics and Optics (1999)
- J. Janszky, Academy Award, Hungarian Academy of Sciences (1999)
- P. Ádám, K. Novobátzky Award, Roland Eötvös Physical Society (1999)
- J. Janszky, Széchenyi Professorship (1998-2001)
- P. Ádám, Széchenyi Professorship (1997-2000)
- T. Kiss, Bolyai Grant (1999-2001)

CONFERENCES:

- *2nd Hungarian-Korean Joint Seminar on Liquid Crystal Science*, Budapest, 4-5 August 1999 (16 participants)
- *International Meeting of the Organic Condensed Matter Division of the Hungarian Physical Society*, Veszprém, Hungary, 26-28 May 1999 (25 participants)

- *14th International Conference on Soft Magnetic Materials* (SMM 14, September 8-10, 1999, Balatonfüred, Hungary (290 participants)
- 2nd *European Conference on Neutron Scattering (ECNS'99)* Budapest, Hungary, September 1-4, 1999 (580 participants)
- *ENSA Committee, European Neutron Round Table, IUPAP Neutron Panel, EU neutron users* meetings. Budapest, Hungary, September 1-4, 1999 (participants)
- *8th International Laser Physics Workshop* (an associated meeting of the World Conference of Science, June 25-July 1, 1999. Budapest) July 2-6. 1999, Budapest.

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