ANNUAL REPORT

2000

MTA SZFKI

RESEARCH INSTITUTE FOR SOLID STATE PHYSICS AND OPTICS

of the Hungarian Academy of Sciences, Budapest, Hungary

ANNUAL REPORT

2000

Host institute of the KFKI Condensed Matter Research Centre

CENTRE OF EXCELLENCE

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

Research Institute for Solid State Physics and Optics
of the Hungarian Academy of Sciences

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ANNUAL REPORT 2000

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

Closed on 1st December, 2000

ISSN 1418-4559

Dear Reader,

It is my pleasure to hand over the Annual Report on the activities of the Research Institute for Solid State Physics and Optics in 2000.

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 our name 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 like X-ray diffraction, NMR-, Mössbauer-, and optical spectroscopy and neutron scattering experiments at the KFKI Research Reactor.

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

In 1999 our institute, together with the KFKI Atomic Energy Research Institute, the KFKI Research Institute for Particle and Nuclear Physics and the Research Institute for Technical Physics and Materials Science established a new organization, the KFKI Condensed Matter Research Centre (CMRC), in order to co-ordinate in the KFKI Campus the research activity in the field of condensed matter physics and applications. Twelve Working Groups belong to the Centre, covering a broad spectrum of condensed matter research. In 2000 the KFKI-CMRC became a "**Centre of Excellence**" within the 5th Framework Programme of the European Union.

Our research activity is financed by the Hungarian Academy of Sciences and by national and international research funds like the Hungarian National Research Fund (OTKA) through supporting individual projects. Since Hungary has joined the EU 5th Framework Programme, the international co-operation has become even more important for the scientific work of our research groups. 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 200 papers in high quality international journals and conference proceedings. The number of publications is somewhat larger than that in the previous years.

The conventional structure of our Annual Report being formed during the last years has been slightly changed in 2000. Two projects in the field of liquid crystal research have been joined together with the name “Liquid Crytals” (Project G). At the same time in the field of laser physics we have started two new projects: “Femtosecond lasers” and “Metal optics” (Project N and O).

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, 2000

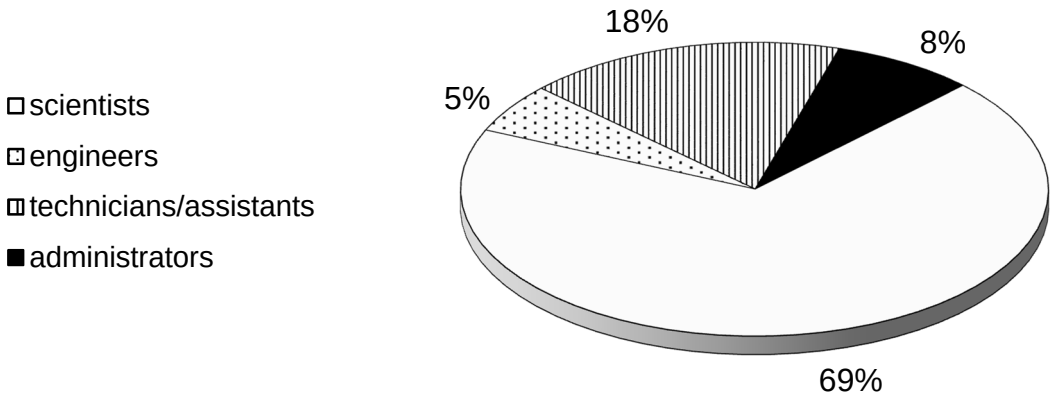
János Kollár

Director

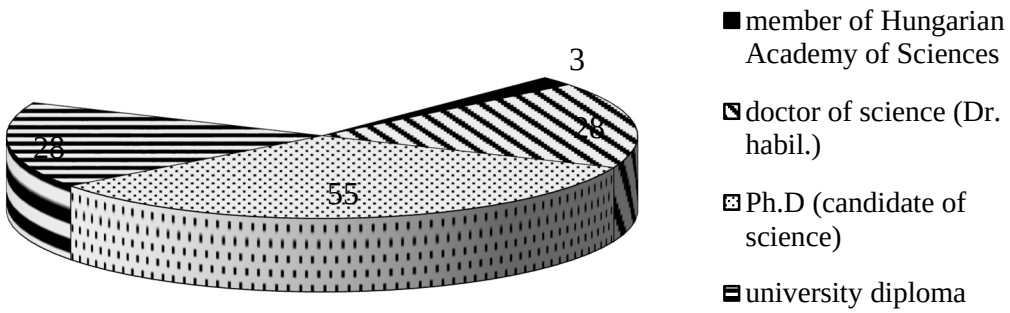
Key figures

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

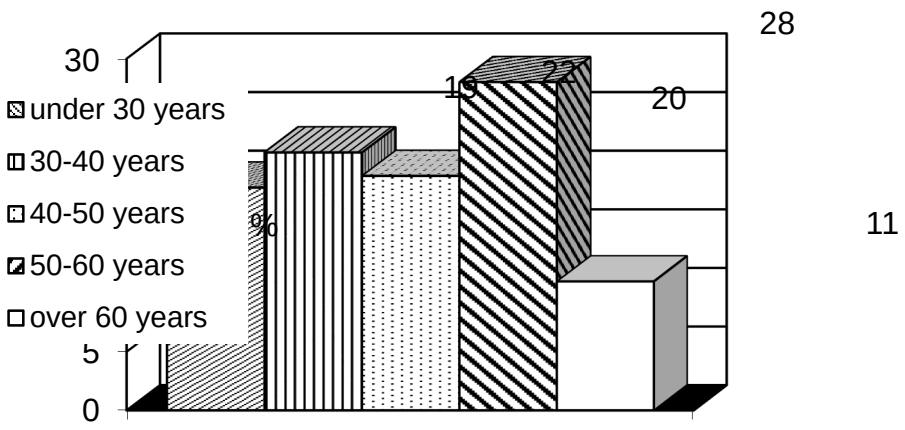
a) by professions:



b) by scientific titles/degrees:

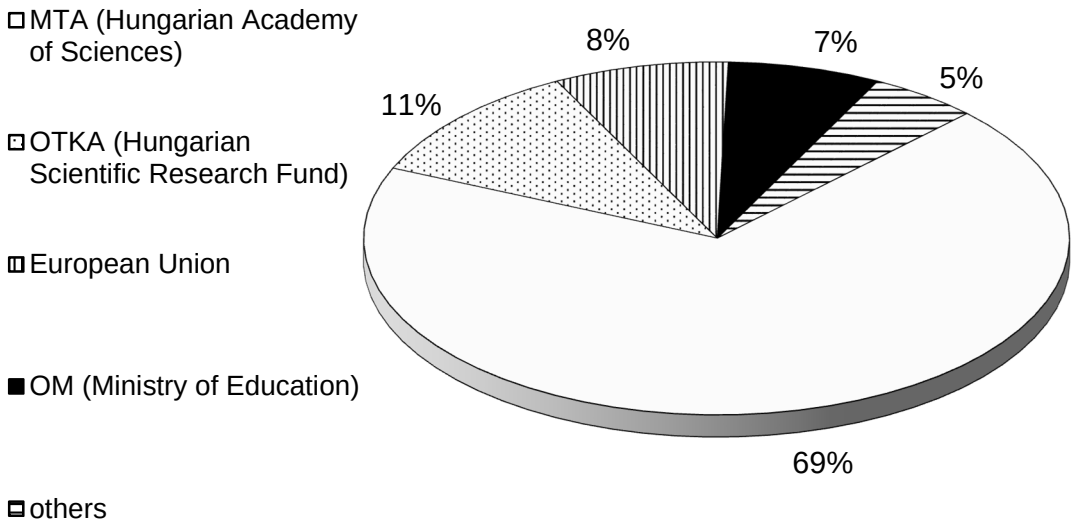


c) by ages:

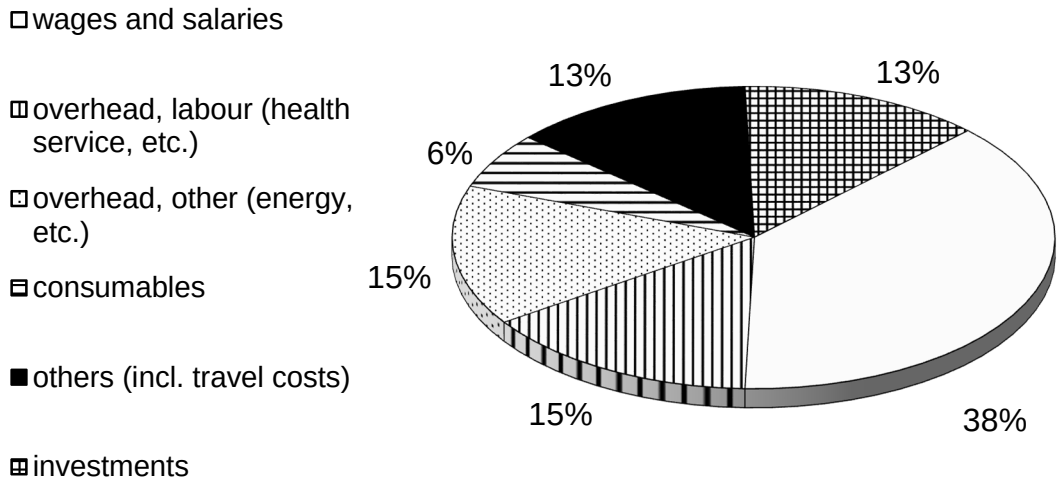


Financial management

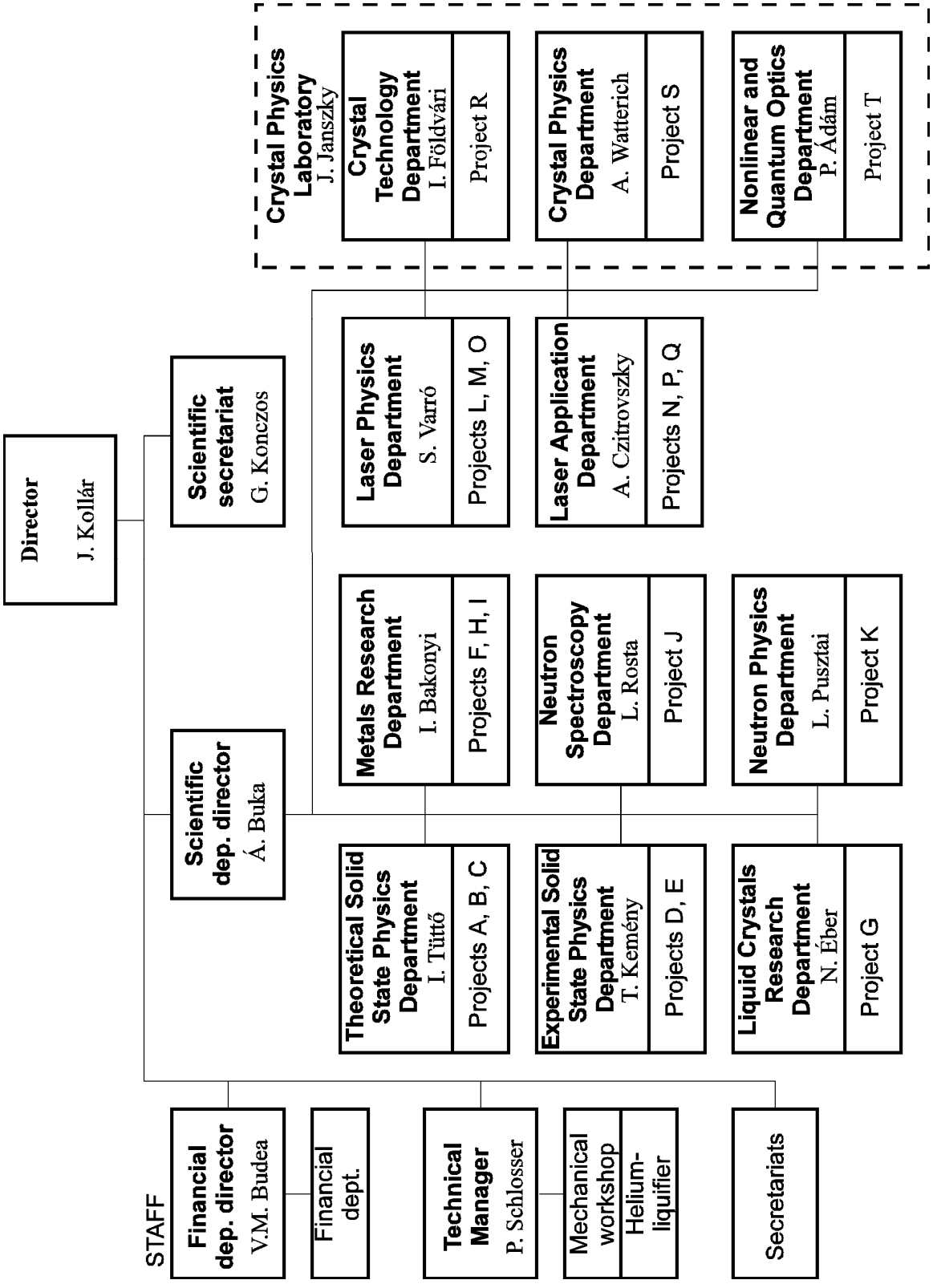
a) Sources of operation costs:



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 studied general spin ladders composed of S=1/2 spins coupled along the rungs, diagonally, and by plaquette interactions. The massive ground state of the conventional two-leg ladder bears close resemblance to the Haldane state of the spin-1 chain. We argued, however, that in case of a ladder one can define two kinds of Haldane states. Both of these possess some kind of topological long-range order, but the two sectors defer in topological quantum numbers, and hence in order parameters. The two topological sector is necessary separated by a phase transition: one cannot move the system from one state into the other in a smooth way. The type of the phase transitions was analyzed by the method of Abelian bosonization. Conclusions were also checked numerically using the density-matrix renormalization group (DMRG) algorithm, which provided a convenient tool to compute topological (string) order parameters in the ground state.

We analyzed the onset of incommensurabilities around the VBS point of the S=1 bilinear-biquadratic spin chain. We proposed a simple effective field theory, which was capable of reproducing all known properties of the commensurate-incommensurate transition at the disorder point q_{vbs}. Moreover, our theory predicted another special point q_{disp}, distinct from the VBS point, where the Haldane gap behaved singularly. The ground state energy density was found to be an analytic function of the model parameters everywhere, indicating that the commensurate-incommensurate transition is not a phase transition in the conventional sense.

We constructed for the first time a spin-1 model on a chain, which has an exactly solvable threefold degenerate ground state. The ground state wave function breaks translational symmetry, thus we have trimerization, Excited states cannot be obtained exactly, but we could determine a few low-lying ones by using trial states, among them solitons.

We are examining the behaviour of the extremly low (O(1/N)) energy excitations of the XXX Heisenberg chain. Strong indications were found that the size of these excitations is of the order of the chain length.

Fermionic models. — In 1995 a momentum-space approach of the DMRG method was developed by Xiang et al., and the ground state energies of the Hubbard model were evaluated. As a conclusion, it turned out, that the accuracy of the new method was worse than the real space version, which delayed its further application in a great extent. We have developed a new code for the momentum space version of DMRG and reproduced White's results for molecules up to 14-20 orbitals. Various additional modifications have been included to increase the efficiency of the method and for the studied system the relative error fell between 10^{-5}-10^{-8}. This novel approach may give a new impetus to solve interacting fermion models in one and two dimensions, as well as in ladder like compounds.

We have investigated the single-particle spectral functions and the density response of a two-band Emery model in the strong coupling limit using analytical and numerical tools. The model describes the almost ideal one-dimensional Cu-O chains

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in the $SrCuO_2$ and Sr_2CuO_3 compounds. We have shown that the low energy hole carriers are the one-dimensional analogs of the Zhang-Rice singlets, and the physics is similar to the one-band Hubbard model. The spectral functions also resemble very much to that of the Hubbard model, with additional weight reduction near the Brillouin zone boundary. This is in agreement with experimental findings.

The transition metal compound $BaVS_3$ shows a wide variety of exotic and yet not well understood features: lowering the temperature, the bad metal becomes insulator with no sign of ordering and presumably with a spin gap at 70 K. A second transition follows at 30 K, where some kind of long-range order is established. Applying pressure, the temperature of the metal-insulator transition decreases, and eventually vanishes at 20 kbar. Near the quantum critical point non-Fermi-liquid (NFL) behaviour is observed with $\rho \propto T^{1.25}$. This is one of the very few observations of NFL behaviour in compounds with *d* electrons. The mostly experimental work, with theoretical input from our side, was done in a close collaboration with the experimental physicist at the Technical University of Budapest and EPFL in Lausanne.

Theory of dissipative notion of heavy particles. — We examined the electron scattering on two level systems in amorphous semiconductors. The infrared divergencies arising in the theory are not completely anomalous to those at the orbital Kondo-effect of metallic case but the TLS-electron coupling transforms similarly to a strong fixed point.

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Grants

OTKA[1] T 017128 Theoretical study of dissipative motion of heavy particles (K. Vladár 1995-2000)

OTKA T 022607 Completely integrable quantum chains (F. Woynarovich 1997-2000)

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

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

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

OTKA D32689 (postdoctoral) Spin and orbital ordering in frustrated vanadium oydes and sulphides. (K. Pencz, 2000)

[1] OTKA=Hungarian Scientific Research Fund

Conference proceedings

A.14. J. Sólyom: Phase diagram of spin ladder models and the topology of short valence bonds. In: *Proc. Open Problems in Strongly Correlated Electron Systems* NATO ARW, Bled 2000, accepted for publication

A.15. K. Penc, W. Stephan*: Spin-charge separation in the Sr_2CuO_3 and $SrCuO_2$ chain materials. In: *Proc. Open Problems in Strongly Correlated Electron Systems*, NATO ARW, Bled 2000, accepted for publication

A.16. P. Fazekas, H. Berger*, L. Forró*, R. Gaál*, I. Kézsmárki*, G. Mihály*, M. Miljak*, K. Penc, F. Zámborszky*: Non-magnetic Mott insulating phase and anomalous conducting state in barium vanadium trisulphide. In: *Proc. Open Problems in Strongly Correlated Electron Systems*, NATO ARW, Bled 2000, accepted for publication

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 non-stationary quantum relaxation of the Ising spin chain in a transverse field of strength *h*. Starting from a homogeneously magnetized initial state the system approaches a stationary state by a process possessing quasi long range correlations in time and space, independent of the value of *h*. In particular the system exhibits ageing (or lack of time translational invariance on intermediate time scales) although no indications of coarsening are present.

We have investigated, mostly numerically, the process $A+A \rightarrow 0$, $B+B \rightarrow 0$ with exclusion between A and B in one dimension. The scaling properties (critical exponents) have been found to exhibit marked deviations from those of standard annihilating random walk and dependence upon the initial conditions (density and composition) has been established and demonstrated by high precision simulations.

We have investigated properties of transient chaos in a chain of dissipative two-dimensional maps, in particular in the critical state.

Quantum systems. — For one dimensional Haldane gap antiferromagnets we proposed a simple effective field theory capable of reproducing all known properties of the commensurate-incommensurate transition at the disorder point. We showed that the ground state energy density and the pair correlation function at fixed distances vary analytically through this transition which is, therefore, not a conventional phase transition.

We studied the ground state of the hard-core Bose gas (spin-1/2 XY model) on regular lattices in arbitrary dimension. We proved that the wave function in coordinate space is strongly nonuniform and derived an approximate expression for it. We gave upper and lower bounds on the ground state energy, and an argument for Bose-Einstein condensation in the ground state.

We have worked out a model including exchange processes for Bose-condensed gases in traps and determined the frequency and damping of the excitations.

The dielectric formalism was generalized for the case of spinor condensates; the density fluctuation and different spin density excitations have been determined.

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[+] Ph.D. Student (University of Szeged)

[++] Permanent position: Loránd Eötvös University, Budapest

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 T029552 Study of atomic systems (P. Szépfalusy, 1999-2002)

OTKA T030543 Mathematical study of systems of quantum spins and particles (A. Sütő, 1999-2002)

DAAD-MÖB 2000/47 Disordered quantum spin systems (F. Iglói, 2000-2001)

Publications

Articles

B.1. G. Palágyi*, C. Chatelain*, B. Berche* and F. Iglói: Boundary critical behaviour of two-dimensional random Potts models. *Eur. Phys. J.* **B13**, 357-367 (2000)

B.2. H. Rieger*, R. Juhász and F. Iglói: Critical exponents of random XX and XY chains: Exact results via random walks. *Eur. Phys. J.* **B13**, 409-412 (2000)

B.3. P. Lajkó* and F. Iglói: Correlation length - exponent relation for the two-dimensional random Ising model. *Phys. Rev. E* **61**, 147-152 (2000)

B.4. F. Iglói, R. Juhász and H. Rieger*: Random antiferromagnetic quantum spin chains: Exact results from scaling of rare regions. *Phys. Rev. B* **61**, 11552-115568 (2000)

B.5. Y-C. Lin*, N. Kawashima*, F. Iglói and H. Rieger*: Numerical renormalization group study of random transverse Ising models in one and two space dimensions. *Progress in Theor. Phys. (Suppl.)* **138**, 479-488 (2000)

B.6. D. Karevski*, L. Turban* and F. Iglói: Conformal profiles in the Hilhorst-van Leeuwen model. *J. Phys.* **A33**, 2663-2673 (2000)

B.7. F. Iglói and H. Rieger*: Long range correlations in the non-equilibrium quantum relaxation of a spin chain. *Phys. Rev. Lett.* **85**, 3233-3236 (2000)

B.8. N. Menyhárd and G. Ódor*: Nonequilibrium Kinetic Ising Models - Phase Transitions and Universality Classes in one dimension. *Brazilian Journal of Physics*, **30**, 113-133 (2000)

B.9. G. Ódor* and N.Menyhárd: Critical behavior of annihilating random walk of two species with exclusion in one dimension. *Phys.Rev. E* **61**, 6404-6414 (2000)

B.10. J. Reidl*, A. Csordás*, R. Graham* and P. Szépfalusy: Shifts and widths of collective excitations in trapped Bose gases determined by the dielectric formalism. *Phys.Rev. A* **61** 043606-1-043606-10 (2000)

B.11. Z. Kaufmann* and P. Szépfalusy: Transient chaos and critical states in generalized Baker maps. *J. Stat. Phys.* **101**, 107-124 (2000)

B.12. P. Szépfalusy and G. Szirmai[*]: Properties of excitations in systems with a spinor Bose-Einstein condensate. *Phys.Rev. A* **61**, 051604-1-051604-4 (2000)

B.13. Z. Kaufmann[*], A. Németh[*], and P. Szépfalussy: Critical states of transient chaos. *Phys. Rev. E* **61**, 2543-2550 (2000)

B.13. A. Sütő: Nonuniform ground state for the Bose gas. *J. Phys. A: Math. Gen.*, accepted for publication

B.14. J. Hajdu[*] and P. Szépfalusy: On the production of entropy within the concept of incomplete description of state. *Annalen der Physik*, accepted for publication

See also A.5.

C. ELECTRONIC STATES IN SOLIDS

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

We have implemented a new method, called **EMTO** (exact muffin-tin orbitals) to calculate the electronic structure of bulk solids and surfaces and combined it with our *full charge density technique*. In this way we have developed an accurate and efficient technique to describe the electronic states in complex systems. We have used the method to perform calculations for **palladium clusters** to show that below a critical size the high surface energy anisotropy stabilizes the icosahedral multiply twinned particle structure against the fcc single crystals. Model structure calculation supports the appearance of ferromagnetic order for non-crystallographic icosahedral symmetry with a small (0.11 μ_B) magnetic moment per atom. These results allow us the interpretation of recent experimental findings [Europhys. Lett., **38**, 195, (1997)] that small free palladium clusters exhibit spontaneous ferromagnetic order.

As another application of the method, the pressure dependent **structural properties of $ScAlO_3$ perovskite** have been determined. Based on the *ab initio* ground state parameters the Debye model was used to compute the phonon contribution to the total free energy. We have found that the $ScAlO_3$ perovskite has orthorhombic structure at 0 K and ambient pressure. This structure is stable relative to the cubic perovskite structure up to pressures of ~ 200 GPa and temperatures of ~ 800 K. The present results support the experimentally observed analogy between $ScAlO_3$ and $MgSiO_3$ perovskites.

In the field of the general development of the density functional theory, we have used the Airy gas model of the edge electron gas to construct an **exchange-energy functional** that is an alternative to those obtained in the local-density and generalized-gradient approximations. Test calculations for rare-gas atoms, molecules, solids and surfaces show that the Airy gas functional performs better than the local-density approximation in all cases and better than the generalized-gradient approximation for solids and surfaces.

We continued the development of the theory of the so-called Polymorphous Coherent Potential Approximation (PCPA). In spite of the success of the PCPA in the structure of random substitutional alloys, it does not treat the charge transfers and related quantities properly. A new PCPA theory was developed which allows a proper treatment of the charge transfers. It was successfully tested for CuZn and CuPd alloys. By applying the methodology of spin-dynamics we are trying to find the long debated ground state of the fcc FeMn and hypothetical fcc Fe, by using the world largest supercomputers.

At ambient pressure, the strongly correlated $3d^1$ system $BaVS_3$ undergoes a phase transition from a bad metal to a non-magnetic Mott insulator at T_{MI} =69K. T_{MI} decreases under pressure or in an external magnetic field. The insulating phase is fully suppressed at T_{cr} =20kbar. $BaVS_3$ offers the opportunity to study the nature of the non-Fermi liquid states, which are adjacent to a spin-gapped Mott insulator.

We have made extensive susceptibility, resistivity and magnetoresistivity measurements on single crystal samples of BaV_3, and discussed the nature of the metal-insulator transition, and of the exotic conducting and insulating states of either

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side of the phase boundary. At p = 1bar, the bad metal is characterized by a critically diverging resistivity and a susceptibility which is essentially that of uncompensated d-electron spins. At $p>p_{cr}$, the resistivity follows $T^{1.25}$ for 1K < T < 40K. The behavior is somewhat similar to that of nearly antiferromagnetic systems, but it cannot be interpreted solely in terms of antiparrallel spin correlations: the non-magnetic nature of the insulator requires the consideration of the orbital degrees of freedom. We find that suppressing the insulator state is synonymous to suppressing the spin gap.

A new method was proposed to calculate the infrared and the Raman spectra of cuprates at the normal state from the measured photoemission spectra. Using the measured one particle spectral function and a phenomenological effective interaction coming from the exchange of paramagnetic fluctuations, we find a self-consistent method to calculate the two particle correlation functions.

We have investigated the **frequency dependent conductivity** of both **superconductors** and **spin density waves** (SDW). We calculated the optical conductivity of Sr_2RuO_4, which is thought to be a p-wave superconductor. We identified strong impurity scattering as a possible source of finite density of states at the Fermi surface even in the superconducting state. We have also determined the microwave conductivity of an SDW in the presence of impurity scattering, and found reasonable agreement with experiment.

We have established the theory of **unconventional SDW** by working out the thermodynamics and the optical properties of this system. Our results are expected to be relevant in a number of cases, when a robust thermodynamic phase transition is observed, but the order parameter can not be found by conventional means (hidden order).

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Annamária Kiss	amk@szfki.hu

Grants

OTKA T23390	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, 1997-2000)

ESF Network program: Electronic structure calculations (J. Kollár, 1998-2002)
DAAD-MÖB 2000/18 Spectroscopical properties of cuprates (I. Tüttő, 2000-2001)

Publications

Articles

C.1. L. Vitos, B. Johansson*, J. Kollár and H.L. Skriver*: Local kinetic-energy density of the Airy gas. *Phys. Rev. A* **61**, 052511-1-4 (2000)

C.2. J. Kollár, L. Vitos, B. Johansson* and H.L. Skriver*: Metal surfaces: Surface, step and kink formation energies. *phys. stat. sol. (b)* **217**, 405-418 (2000)

C.3. L. Vitos, H.L. Skriver*, B. Johansson* and J. Kollár: Application of the exact muffin-tin orbitals theory: the spherical cell approximation. *Comp. Mat. Sci.* **18**, 24-38 (2000)

C.4. L. Vitos, B. Johansson*, H.L. Skriver* and J. Kollár: Stability of fcc (110) transition and noble metal surfaces. *Comp. Mat. Sci*. **17**, 156-159 (2000)

C.5. H.L. Skriver*, A.V. Ruban*, J.K. Norskov*, L. Vitos and J. Kollár: Steps, kinks and segregation at metallic surfaces. *Prog. Surf. Sci.* **64**, 193-198 (2000)

C.6. L. Vitos, B. Johansson*, J. Kollár and H.L. Skriver*: Exchange energy in the local Airy gas approximation. *Phys. Rev B* **62**, 10046-10050 (2000)

C.7. L. Vitos, B. Johansson*, and J. Kollár: Size-dependent paramagnetic-ferromagnetic phase transition in palladium clusters. *Phys. Rev. B* **61**, R11957-60 (2000)

C.8. B. Újfalussy, J.S. Faulkner*, N.Y. Moghadam*, G.M. Stocks* and Y. Yang*:: Calculating properties with the polimorphous coherent potential approximation. *Phys. Rev. B* **61**, 12005 (2000)

C.9. N.N. Lathiotakis*, B.L. Gyorffy* and B. Újfalussy: First principles Asymptotics for the Oscillatory Exchange Coupling in Co/Cu/Co of (100), (110) and (111) orientations. *Phys. Rev. B* **61**, 6854-6865 (2000)

C.10. M. Opel*, R. Nemetschek*, C. Hoffmann*, R. Philipp*, P.F. Müller*, R. Kackl*, I. Tüttő, A. Erb*, B. Revaz*, E. Walker*, H. Berger*, L. Forró: Carrier relaxation, pseudogap and superconducting gap in high-T_c cuprates: A Raman scattering study. *Phys. Rev B* **61**, 9752-9774 (2000)

C.11. B. Dóra, A. Virosztek and K. Maki*: Optical conductivity of the p-wave superconductor Sr_2RuO_4. *Physica C* **341-348**, 775-776 (2000)

C.12. A. Virosztek, B. Dóra and K. Maki*: Microwave conductivity in spin density waves. *Ferroelectrics,* accepted for publication

C.13. B. Magyari-Köpe, L. Vitos and J. Kollár: Ab initio study of structural and thermal properties of $ScAlO_3$ perovskite, *Phys. Rev. B*, accepted for publication

C.14. P. Fazekas: Spin and Orbital Order in Itinerant Ferromagnets. *Foundations of Physics*, accepted for publication

Books, book chapters

C.15. J. Kollár L. Vitos and H.L. Skriver*: From ASA towards the full potential, in Electronic Structure and Physical Properties of Solids. The Uses of the LMTO Method. *Lecture Notes in Physics*, **535**, Ed. H. Dreysse, Springer, pp 85-113 (2000)

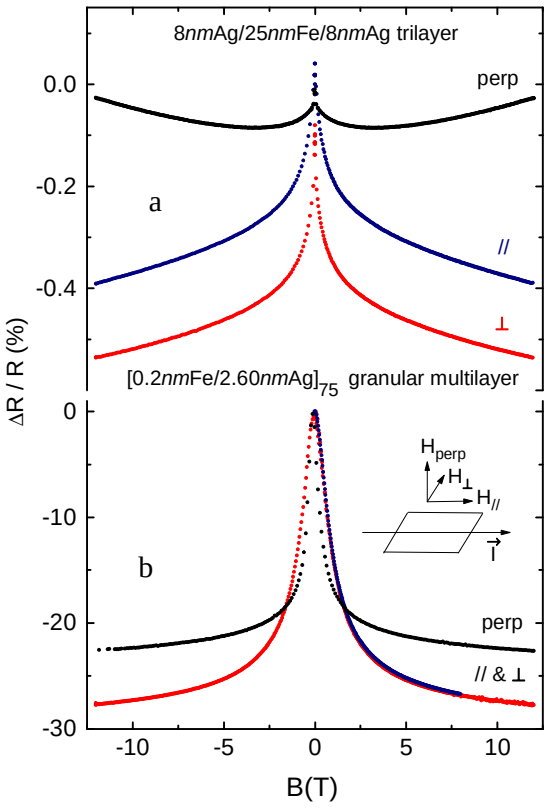
See also A.9., A.10., A.16.

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. – Recently, a class of nanocrystalline alloys with composition $Fe_{44}Co_{44}Zr_7B_4Cu_1$ has been developed, which are capable of operating at higher temperatures and have good soft-magnetic properties. They are promising as high-temperature magnetic applications, e.g. as rotors in electric aircraft. We performed a systematic study of slightly different composition nanocrystalline alloys with higher Fe-Co content [$(Fe_{1-x}Co_x)_{90}Zr_7B_2Cu_1$ ($0 \le x \le 0.6$)] and, consequently, with higher saturation magnetization, which is one of the key intrinsic magnetic properties. The nanocrystalline alloys were prepared by a heat treatment up to the first crystalline stage of the respective amorphous ribbons. The nanocrystalline state and the grain sizes of the nanosize ferromagnetic *bcc* precipitates embedded in the ferromagnetic residual amorphous phase were determined by X-ray diffraction and it was found that the about 25 nm grain size did not change significantly with composition. Co was preferentially partitioned to the residual amorphous phase, and the *bcc* grains were accordingly enriched by Fe according to the ^{57}Fe Mössbauer spectroscopy results. The room-temperature coercive field measured by a superconducting quantum interference device magnetometer increased with the Co addition, which is attributed to the increasing magnetostriction constant in line with the behaviour found in bulk Fe-Co alloys. In our samples the largest saturation magnetization with modest increase of the coercive field was found for concentrations between $Fe_{72}Co_{18}Zr_7B_2Cu_1$ and $Fe_{63}Co_{27}Zr_7B_2Cu_1$, and the Curie point of the residual amorphous phase is estimated to be the highest for this latter composition, which seems to be optimal for high-temperature soft-magnetic applications.

Magnetoresistance of Ag-Fe multilayers. – By studying the magnetoresistance of trilayers containing a single magnetic layer it is possible to separate the contribution of a single interface. The trilayer and multilayer samples were prepared on Si single crystal substrate at room temperature by vacuum evaporation in a base pressure of 10^{-7} Pa. Magnetoresistance curve of an (as deposited) 8 nm Ag \ 25 nm Fe \ 8 nm Ag trilayer measured in parallel, transversal and perpendicular magnetic field alignment up to 12 T magnetic field is shown in the figure (a). $R_{//}$ and $R_{\perp}$ show similar and rather unusual magnetic field dependence in the high field region. (The two curves are shifted



Magnetoresistance measured at 4.2 K for three different magnetic field alignments as indicated in the figure.

relative to each other because of a small anisotropic magnetoresistance below 0.2T.) The equal decrease of the parallel and the transversal magnetoresistance and the absence of saturation up to 12 T magnetic field has not yet been observed on a single ferromagnetic Fe layer. On the other hand the cusp like shape of the magnetoresistance curve and the extremely high saturation field is typical of the giant magnetoresistance (GMR) in granular systems. Magnetoresistance of a Fe-Ag sample which has a [2.6 nm Ag+0.2 nm Fe]$_{75}$ nominal layer structure is shown in the figure (b). In this sample the thin Fe layers are not continuous and it shows characteristics of a granular system, e.g. it is superparamagnetic with a blocking temperature around 40 K. The observed magnetoresistance of the trilayer sample (a) is attributed to a granular interface structure. By heat treating the sample at adequate temperature the nonequilibrium granular interface alloy decomposes and the normal (positive) high field magnetoresistance is observed. The existence of a granular interface magnetoresistance raises the question how this term is related to the magnetoresistance arising from interlayer coupling in case of multilayers. Our studies demonstrated that the granular interface contribution is dominant in Fe/Ag multilayers. By investigating Cr/Fe/Cr trilayers it was also shown that the granular interface magnetoresistance is not restricted to immiscible elements.

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Grants

OTKA T 030753	Magnetic systems with nanoscale inhomogeneities (I. Vincze, 1999-2002)
OTKA T031854	The influence of atomic volume and local environment to the anomalous magnetic properties of equiatomic alloys (T. Kemény, 2000-2003)
AKP[2] 98-25 2,2	The relation of magnetic properties and the grain structure in nanocrystals (T. Kemény, 1999-2000)

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D.1. 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* **61**, 4109-4116 (2000)

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[2] AKP=Research Grant of the Hungarian Academy of Sciences

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See also F.1., I.13.

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. Beside the phototransformation non-ambient conditions can also lead to new polymer phases. In order to map the phase diagram of C_{60} polymers we made model calculations based on density functional theory. These theoretical works were extended by far-infrared vibrational studies of high-pressure-high-temperature C_{60} polymers and the C_{60} dimer. Further, we have worked out the production of phototransformed C_{60} in gram quantities and isolated its cycloadduct dimer component in spectroscopically pure form. Besides the dimer we extracted a mixture of soluble higher oligomers from the raw photopolymer. The separation and purification of the oligomers are in progress.

X-ray holography with atomic resolution - In holography, the scattered radiation is mixed with a reference wave and the resulting interference pattern is recorded. The hologram contains both the intensity and the phase information and the 3 dimensional image of the object can be reconstructed. 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 technique usable in practice further developments are necessary. First of all the data acquisition time has to be decreased. Therefore we implemented this method at synchrotron sources. This resulted in measuring times in the range of 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. A further limitation is the capability of imaging heavy atoms only. This comes from the low scattering power of the light atoms.. After holographic reconstruction, the strength (or brightness) of the atoms are proportional to the square of their atomic number (Z) and also with r^{-1} where r is the distance from the central atom. Therefore to see an atom with low Z or being far, the holographic oscillations have to be measured with much higher precision than in previous works. We solved the above problem and demonstrated experimentally the capability of imaging light atoms. An example is shown in Fig.1.

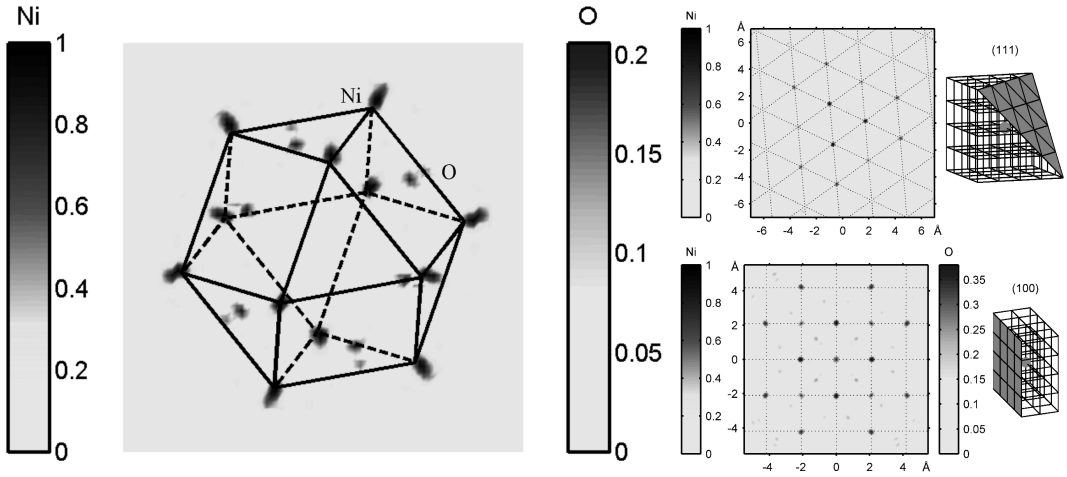

Fig.1. The holographically reconstructed 3D image of Ni and O atoms in a NiO sample (left panel), and selected atomic planes of the same sample (right panel).

Theory of phase transformations. — We investigated vapor condensation and freezing in the framework of continuum models and cluster dynamics calculations.

Starting from an exact gradient transcription of the perturbative density functional theory of homogeneous vapor condensation, we proposed an analytical approximation that reproduces the density profile and free energy of critical fluctuations to high accuracy. For a broad variety of substances, the new method predicts nucleation rates that are orders of magnitude closer to experiment than those from the classical approach.

A quantitative test of the kinetic Turnbull-Fisher model has been performed by numerically solving the master equations that describe the time evolution of cluster population. Evaluating the kinetic and interfacial parameters from nucleation data on oxide glasses, we calculated the macroscopic growth rates and compared with experiments. We demonstrated the inadequacy of microscopic kinetic parameters in describing macroscopic growth, a finding that could not be explained by either the curvature dependence of the interfacial free energy or the self-consistency correction for the cluster free energy.

Nucleation and growth of stable and metastable phases have been studied in the framework of Cahn-Hilliard type theories relying on two and three-well free energy-order parameter relationships composed of three parabolas. Analytical solutions were presented for the free energy of critical fluctuations and the growth rate. In the case of metastable solidification, it has been found that above a bifurcation temperature the interface is layered; a metastable layer is sandwiched between the initial and the stable phases. Above this temperature, two solutions exist, one with a sharper interface and another with an extended metastable layer, of which the latter has a larger free energy. Below the bifurcation point, only the metastable phase is able to nucleate directly from the liquid.

In cooperation with team H, we investigated the dynamic response of dendritic solidification to spatially homogeneous time-periodic forcing. Our phase-field simulations indicate that the frequency of dendritic side-branching can be tuned by oscillatory pressure or heating and that besides the side-branching mode synchronous with external forcing, modes which oscillate with higher harmonic frequencies are also

present with perceptible amplitudes. These results have been confirmed by experiments performed on liquid crystals. We explored binary nucleation and growth in the framework of the phase-field theory (Fig. 2).

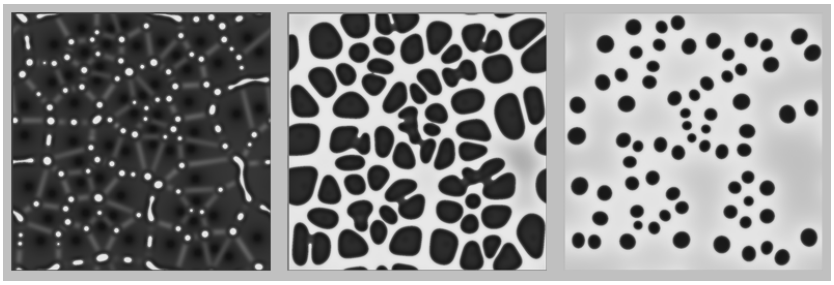

Fig.2. Snapshots of two-dimensional isotropic phase-field simulation of crystallization in an ideal binary alloy. The pictures from left to right correspond to initial compositions x = 0.2, 0.5, and 0.8, where $x = (c - c_s) / (c_l - c_s)$*, while* c_l *and* c_s *are the liquidus and solidus compositions, respectively. The gray tones indicate the local composition (black and white correspond to the solidus and liquidus compositions, respectively). Note the depletion zone around particles and the non-spherical shapes at the late stages evolving due to the interaction of the diffusion fields of individual particles.*

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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)

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MTA-NSF International Grant No. 108 (K. Kamarás, J.L. Musfeldt*, 1998-2000)

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see also D.3., D.9., G.17. G.18.

F. ELECTRON CRYSTALS

G. Kriza, P. Matus, L. Németh, I. Pethes, B. Sas

Dissipation in high-critical-temperature superconductors. — In classical Type II superconductors, the main source of dissipation in the presence of high transport currents has been demonstrated to be the motion of Abrikosov vortices. The experimental hallmark of this mechanism is the Bardeen-Stephen law predicting a vortex-motion resistivity proportional to the magnetic field. In high-T_c superconductors, experimental evidence for the Bardeen-Stephen law is restricted to a small high-temperature portion of the superconducting part of the temperature–magnetic field phase diagram. We have studied the temperature- and magnetic field evolution of the voltage–current characteristics in $Bi_2Sr_2CaCu_2O_8$ single crystals using short current pulses. We find that at low temperatures, in the vortex solid phase, the differential resistance saturates at high currents at a value which is both temperature and magnetic field independent, in sharp contrast with the Bardeen-Stephen law. We consider the effects of fluctuations of the superconducting order parameter between the superconducting planes and extended quasiparticle states in *d*-wave superconductors in order to interpret this surprising result.

Pseudogap in quasi-one-dimensional metals. — Thermal fluctuations in highly anisotropic metals are strongly enhanced compared to their isotropic counterparts. Precursor fluctuations of low-temperature correlated states are observed over a broad range of temperature. The fluctuating order parameter causes a depletion of the density of states near the Fermi energy, a situation often described as the opening of a "pseudogap." We have studied the magnetic susceptibility and nuclear spin-lattice relaxation rate in the high-temperature "normal" and low-temperature charge density wave states of the quasi-one-dimensional compound $(TaSe_4)_2I$. Both quantities are strongly temperature dependent in the normal phase and the singularity at the three-dimensional ordering is much weaker than predicted by mean field theory. We ascribe these finding to the opening of a pseudogap well above the CDW temperature. The temperature dependence of the pseudogap is inferred from the data. The absence of a Hebel-Slichter type coherence peak in the charge density wave phase is also explained by the pseudogap in the normal phase.

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Grants

OTKA T023786	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)

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Articles

F.1. B. Sas, F. Portier*, K. Vad*, B. Keszei*, L.F. Kiss, N. Hegman*, I. Puha*, S. Mészáros*, F.I.B. Williams*: Metastability line in the phase diagram of votices in BiSrCaCuO. *Phys. Rev. B* **61**, 9118-21 (2000).

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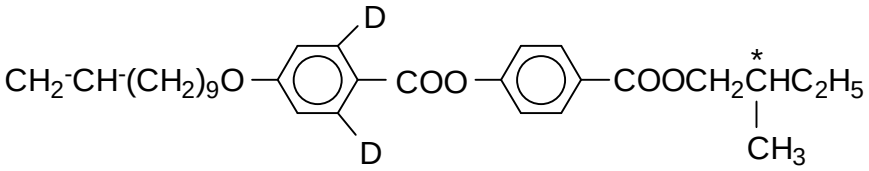
F.4. L. Németh, P. Matus, and G. Kriza: Nuclear magnetic resonance in the pseudogap- and charge-density-wave states of $(TaSe_4)_2I$. *Synthetic Metals,* accepted for publication.

G. LIQUID CRYSTALS

Á. Buka, L. Bata, E. Benkler, T. Börzsönyi, N. Éber, K. Fodor-Csorba, A. Jákli, I. Jánossy, E. Szabó, T. Tóth-Katona, A. Vajda

Synthesis and miscibility studies. — A deuteration procedure was developed for the preparation of a monomeric liquid crystal (S)-4-[(2-methylbutyloxycarbonyl)-phenyl]-4-n-(10-undecenyloxy)benzoate-d_2 (MBUB-d_2). Molecular dynamics studies of this compound by ^{2}H NMR showed an unusual behaviour, the tumbling motion of the molecules was quicker than their spinning.



MBUB-d_2

A compound with higher deuterium content, MBUB-d_4, was also prepared in larger quantity for the synthesis of new deuterium labelled chiral liquid crystalline polysiloxanes possessing smectic C^* phase in a wide temperature range (-15 °C — +60 °C). Their orientational order was determined by ^{2}H NMR spectroscopy.

The phase sequences of a new chiral homologous series (Qm n/m) (S)-[4-n-alkyloxybenzoyloxyphenyl]-4'-[(2-n-alkyloxy)propionyloxy]benzoate were determined by polarizing microscopy and DSC. All members showed enantiotropic N^* and SmC^* mesophases with a spontaneous polarization about 120 nC/cm^2. The compounds were used for preparing room temperature enantiotropic ferroelectric binary mixtures.

Pattern formation. — *Oscillatory shear induced instabilities:* Slow precession of the director has been generated by elliptic shear applied to a homeotropically oriented nematic above the electric bend Fréedericksz transition (FT). The character of the accompanying non-linear waves changes from diffusive phase waves to dispersive ones exhibiting spirals and spatiotemporal chaos as the FT is approached from above. An exact solution of the flow alignment equations captures the observed precession and predicts its reversal for non-flow-aligning materials. The FT transforms into a Hopf bifurcation opening the way to understand the wave phenomena.

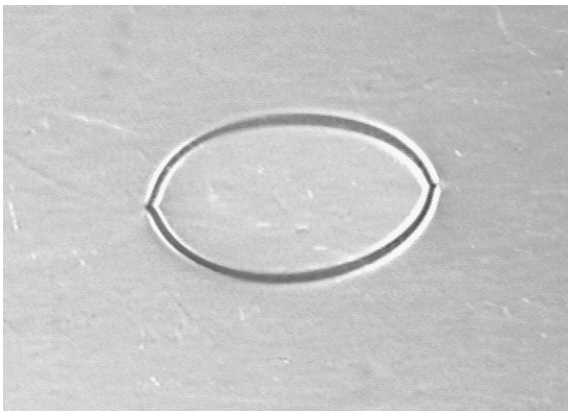
Nematic - smectic B interface: Phase-field calculations performed in two dimensions (2D) and experiments on thin (quasi-2D) liquid crystal layers show that the frequency of dendritic side-branching can be tuned by spatially homogeneous time-periodic forcing (i.e., by oscillatory pressure or heating). It has been demonstrated that in addition to the side-branching mode synchronous with external forcing as emerging from the linear Wentzel-Kramers-Brillouin analysis, modes that oscillate with higher harmonic frequencies are also present with perceptible amplitudes.

Viscous fingering: Lateral undulations have been observed in the fingers at the air – nematic interface by periodically switching on and off the electric field, which reorients the nematic and thus changes the viscosity, the surface tension and its anisotropy (mainly enforced by a single groove in the cell). These undulations correlate with the switching frequency, as well as with tip velocity oscillations which

is maximal at the smallest curvature. The oscillations appear to be decoupled from spontaneous (noise-induced) side branching. We conclude that the lateral undulations are generated by successive relaxations between two limiting patterns controlled by the change in the anisotropy. This scenario is confirmed by numerical simulations in the linear geometry, using a phase field model for anisotropic viscous fingering.

Electrohydrodynamic instabilities: A periodic structure (prewavy pattern) appears below the onset of electroconvection in a homeotropically aligned nematic liquid crystal. It is characterized by periodic modulation of the director in the xy-plane, which can be distinguished from electroconvection patterns with modulation in the xz-plane. The phase diagram of the instability in the frequency-voltage plane, the voltage and frequency dependence of the azimuthal rotation angle and the wavelength of the prewavy pattern were determined. This prewavy pattern always evolves into chevrons above the onset of convection. The wavelength of the chevrons and the orientation of their alternating zigzag rolls depend on the director distribution of the prewavy pattern.

Non-linear optics. — Optical reorientation of nematic liquid crystals was measured in the presence of various isomerizable dyes. The anomalous angular dependence of the reorientational nonlinearity was observed for three different dye-dopants. In order to extend the accessible angular range in these measurements, a new technique was developed, which made possible to measure the amplification of the optical torque in planar cells. The method is based on optical generation of inversion walls in liquid crystal cells.



Inversion wall forming a loop generated by a laser beam in a nematic liquid crystal cell. The director rotates by 180º across the wall.

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Grants:

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

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

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

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

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

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

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

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

OTKA N-31165, MTA-OTKA-NSF (Hungarian-USA bilateral): Optical alignment of liquid crystals (István Jánossy, 1999-2001)

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

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G.32. 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* **105**, 505-511 (1999)

G.33. A. Jákli, G.G. Nair*, Y. Huang*, W. Cao*, L.-C Chien*: Chirality and electro-optics of banana-shaped materials. *Technical Reports ALCOM Symposium*, Vol. **IX**, 35-40 (2000)

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See also E.23, E.28

H. METAL PHYSICS

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

Metal-hydrogen systems. — In the ^{1}H NMR study of $\mathbf{Zr_y(Ni_{1-x}Cu_x)_{1-y}\text{-}H}$ amorphous alloy-hydrogen systems several NMR characteristics, namely the low-temperature ("rigid-lattice") spectrum shape and second moment (M_2), and the spin-spin (T_2) relaxation time, have been measured and interpreted. These results show local fields originating from a few proton neighbours, contrary to the "lattice gas"-like continuous hydrogen distribution model. The 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. The interpretation of the other NMR parameters, that is, the spin-lattice relaxation time (T_1) and the line shift terms (Knight shift and chemical shift) is in progress, and the expected conclusions will reflect the electronic structure of these metallic systems.

High purity $\mathbf{Pd_{1-x}Ag_x}$ (x=0.1; 0.2 and 0.35) alloys prepared in our laboratory were charged with hydrogen, and the in-situ-NMR spectrum, T_1 and T_2 relaxation time and electrical resistivity measurements were continued and partly published on this fcc crystalline alloy system which is considered as a model material representing a chemically disordered system for the hydrogen storage materials. The in-situ resistivity and NMR measurements give a unique chance for the investigation of non-equilibrium hydrogen charging, discharging and diffusion processes, in addition to the common equilibrium measurements. The two commonly used charging methods, namely the gaseous and electrolytic methods were used. Both kinds of experiment were carried out under equilibrium and non-equilibrium conditions, too. As a first illustration, the H-content measured by NMR during charging and discharging processes and the charging/discharging rate are shown in Fig. 1.

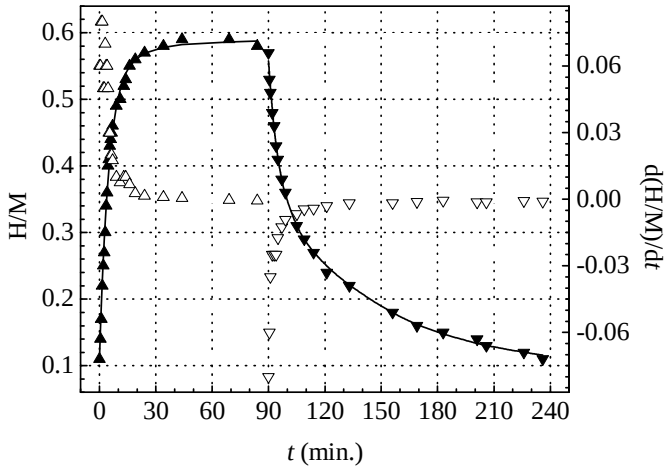

Figure 1. Time dependence of hydrogen charging (up triangles) and discharging (down triangles) of $Pd_{0.9}Ag_{0.1}$ at T = 353 K. Open symbols: charging and discharging rates.

As a second illustration, the resistivity change during the two processes is shown in Fig. 2. The resistivity decrease during the first part of H charging and the hysteresis of that during a charging-discharging cycle seems to be a good challenge for the complete understanding of the non-monotonic time dependence.

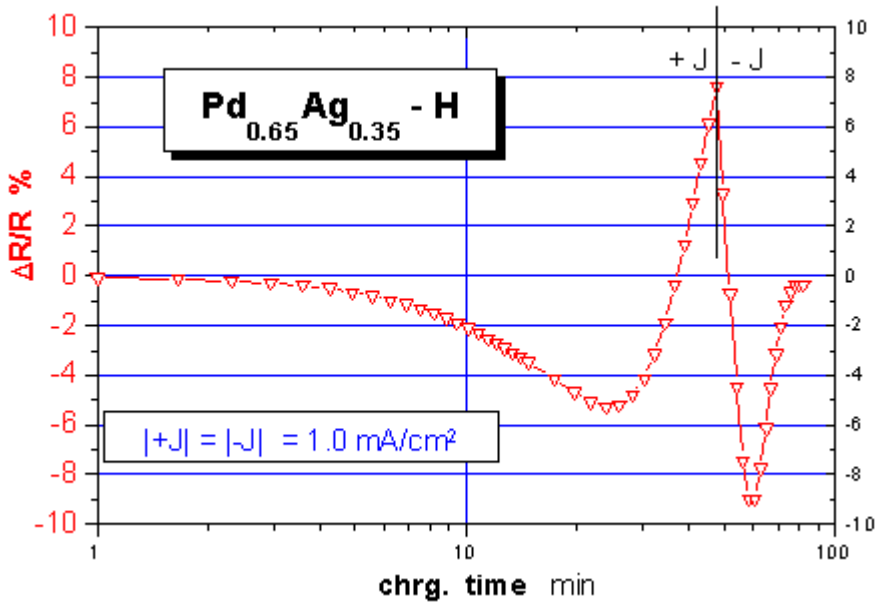

Figure 2. Resistivity change during the charging (+J) and discharging (-J) processes in a Pd-Ag-H alloy

Transition metal complexes. — An extensive analysis of the ^{1}H and ^{19}F NMR line shapes of $[M(1\text{-ethyl-1}H\text{-tetrazole})_6](BF_4)_2$ compounds (M = Fe or Zn) was carried out between room temperature and 2.2 K and the results were interpreted in connection with conclusions based on spin-lattice relaxation time (T_1) measurements. Irregular behavior of ^{1}H data was found in the temperature range 70 K - 120 K that suggests the presence of a phase transition involving molecular group reorientation-type motions becoming active/inactive. An analysis of T_1 data of this ethyl and of the similar methyl complexes provided thermodynamic data on the molecular group reorientation type motions present in certain temperature regions and on the electron spin relaxation for the iron complexes.

Hydrogen in steel. — This work is related to an industrial test applied in characterization of enamel-grade steel plates prior to the enameling procedure. The conventional test is based on an electrochemical permeation technique and the observation of hydrogen at the exit side of the sample. However, this standard test is known to fail if the sample contains some alloying elements (Ti, B etc.), if the thickness of the sheet is very small or large, etc. The aim of our work is to elaborate a procedure that is reliable for essentially all types of steel samples used in the enamel industry nowadays, and makes it possible to determine the diffusion coefficient of hydrogen and the trap concentration with a single measurement. Besides the experimental work, we deal with numerical simulation to elucidate the effect of traps on the experimental permeation curves.

Metastable metallic phases. — Differential scanning calorimetry (DSC) and X-ray diffraction measurements (XRD) were performed on a melt-quenched $Fe_{40}Ni_{40}P_{14}B_6$ amorphous alloy in order to study the influence of different heat treatments (linear heating and isothermal annealing). In both cases, the amorphous-crystalline transition

was found to take place in one step and a nanocrystalline state consisting of fcc-(Ni,Fe) and $(Ni,Fe)_3(P,B)$ phases formed. Since the enthalpies released during the amorphous-nanocrystalline transformations were very similar in both cases, it can be concluded that the linear heating and the isothermal annealing of the as-quenched amorphous state yield energetically similar states. The X-ray diffraction results, on the other hand, showed that the average grain-size values after the nucleation and growth process are by a factor of 2 larger in the case of linear heating. It is well known that an assembly of fine grains exhibits a contribution to the total stored energy originating from the grain boundary region. This means that the smaller the average grain size, the larger the total grain boundary energy, i.e., isothermal annealing would have been expected to result in a larger energy released than during linear heating, under the usual assumption of constant specific grain boundary energy. The discrepancy described above can be eliminated by taking into account the difference in the microstructures developing during the different heating routes. Previous studies including TEM investigations have revealed that in the case of the Ni-P binary system, isothermal and linear heating result in completely different microstructures with different grain boundary energies. The microstructure formed during isothermal annealing is characterized by the well-known barrel-shaped crystallites containing an ordered and oriented lamellar structure on a nanometer scale. On the other hand, linear heating results in a homogenous random mixture of fcc-Ni and tetragonal Ni_3P-type grains with a high grain boundary energy of the Ni-Ni_3P and Ni_3P-Ni_3P interfaces. The results of the present study seem to indicate a similar situation for the crystallization of the $Ni_{40}Fe_{40}P_{14}B_6$ amorphous alloy as well.

Metallic multilayers. — Direct-current plating, pulse-plating, two-pulse plating and reverse-pulse plating were used to produce electrodeposited Co-Cu alloys and Co-Cu/Cu multilayers under galvanostatic control from an electrolyte containing $CoSO_4$ and $CuSO_4$. Atomic force microscopy, X-ray diffraction and transmission electron microscopy were used to study the sample structure and morphology. Direct-current plating resulted in a $Co_{95}Cu_5$ alloy with nearly equal amounts of fcc and hcp phases, while all pulsed-current methods yielded multilayers with fcc structure. Giant magnetoresistance (GMR) behavior was observed in the multilayers with a maximum MR ratio of about 9 % as measured at 8 kOe. The shape of the MR curves and the magnitude of the GMR were very similar, regardless of the sign of the current between the Co-deposition pulses. The results of structural studies also confirmed the formation of a multilayer structure for each pulsed electrodeposition mode. The conclusion was that the spontaneous exchange reaction between Co and Cu^{2+} is responsible for the formation of a pure Cu layer even under reverse-pulse plating conditions. The GMR of the multilayer deposits decreased with increasing bilayer number, due to the deterioration of the microstructure as the deposit grew.

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Grants

OTKA T 022 124	Preparation and investigation of single-phase nanocrystalline metals (I. Bakonyi, 1997-2000)
OTKA T 031994	Random walk and diffusion of hydrogen in alloys (K. Tompa, 2000-2002)
OTKA F 032046	Preparation of metallic multilayers from compositionally modulated flowing electrolytes (L. Péter, 2000-2003)
BAYATI[+]	Contract for "Diffusion and solubility study of hydrogen in IF steels" (L. Péter, 2000)

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I. 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. — In an effort to have a better understanding the structure – properties relationship in soft magnetic nanocrystalline alloys, we have developed a new model to simulate the experimentally observed temperature evolution of the initial susceptibility in the coupled ferromagnetic state of nanocrystalline alloys. An extension of the random anisotropy (Herzer) model was used by taking into account two new anisotropy terms besides the magneto-crystalline term of the nanograins: the non-averaging local anisotropy of the residual amorphous matrix and the magnetostatic energy arising from the difference between the saturation magnetizations of the two phases. The first term decreases while the latter term increases as the measuring temperature approaches the Curie temperature of the amorphous phase, giving rise to a minimum in the overall anisotropy and a corresponding maximum in the permeability (Hopkinson peak). It could be shown that the Hopkinson peak, which is progressively rounded off and displaced to lower temperatures as the nanocrystallization proceeds, can be perfectly described by using the amount of the crystalline phase as determined by quantitative X-ray diffraction (XRD), the only fitting parameter being the effective demagnetizing factor of the nanograins.

In investigating the role of the residual amorphous matrix in determining the temperature dependence of soft magnetic properties, a large (more than 300 K) increase of the decoupling temperature (T_c^{am}) was found with increasing crystalline fraction in Nanoperm type alloys (Fig. 1). This is in contrast to the Finemet alloys where T_c^{am} varies by a few tens of Kelvin only around the original, as-cast amorphous T_c value when the amount of crystalline fraction is increased by appropriate annealing.

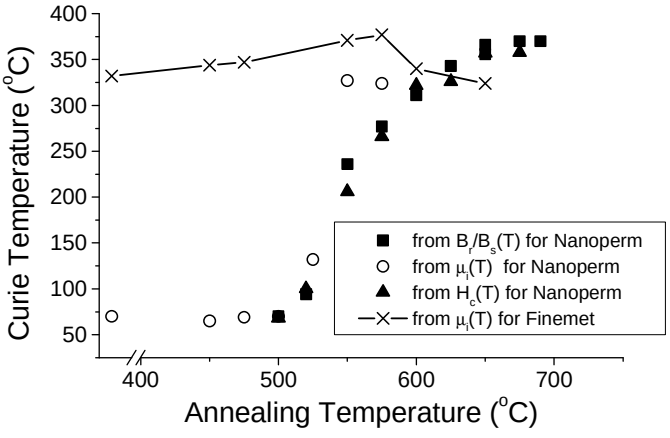

Fig.1. Evolution of the Curie temperature of the residual amorphous matrix as a function of heat treatment, determined from the permeability kink point of ribbon shaped samples. For Nanoperm, the values determined from the hysteresis loop are also presented.

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Using these fundamental results, a nanocrystalline ribbon core was developed, tested and applied as a common mode choke. At present, we are preparing the mass production of these cores. This work was centered around the tasks of our NATO Science for Peace program aimed at preparing soft magnetic nanocomposites for audio and radio frequencies.

Scanning electron microscopy. — In performing materials research studies, the laboratory's facilities have been developed in the following areas: (i) a new sample preparation method has been introduced enabling us to investigate the magnetic domain structure of polycrystalline samples by SEM, (ii) the ion beam sample thinning system was applied to biological samples and (iii) the X-ray microanalysis measurements were extended to glass furnace technology investigations.

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Grants

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)

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See also H.7., H.11.

J. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

L. Rosta, L. Almásy, M. Avdeev, S. Borbély, L. Cser, J. Füzi, A. Len, E. Rétfalvi, L. Riecsánszky, Gy. Török

The Neutron Spectroscopy Department is one of the Laboratories of the associate Institutes forming the Budapest Neutron Centre, which operates the 10 MW Budapest Research Rector (BRR) and its experimental facilities 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 cold neutron guide system. Our 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 year 2000 a major step in upgrading of the experimental possibilities was made: the installation of a cold moderator was performed for expanding our condensed matter research possibilities for the highly demanded *cold neutron* region. This liquid hydrogen cold neutron source has been assembled and commissioned. For the improved transportation of the neutron beams a major part of the neutron guide system was replaced by modern optimised supermirror guides. Besides this major instrument development programme, various scientific 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 ILL-Grenoble, HMI Berlin, FLNP (Russia), PSI (Switzerland) or LLB Saclay (France) where we took part in the construction of the Spin-Echo spectrometer (MESS).

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

Liquids. — Binary and ternary liquid mixtures were studied by small-angle neutron and X-ray scattering, the two main components being water (heavy water) and an organic solute (pyridine, 2-,3-, and 4-methyl pyridines, acetonitrile and tetrahydrofurane), and the third components were various chloride salts in the aqueous solutions of methylpyridines. In the three-component solutions the influence of the different cations on the size of the immiscibility region and the critical exponents were investigated. The expansion or the shrinkage of the immiscibility loop could not be simply related to the change of a single parameter, the size or the

charge of the cation. For the binary solutions the experimentally determined characteristic parameters of the nonideal mixing - the concentration and density fluctuations were compared to the results of thermodynamical calculations using the Kirkwood-Buff theory. The use of an additional experimentally accessible parameter - the correlation length – made it possible to obtain information about the structure of the liquid around the solute, the estimation of the microscopic structure of the liquid around the solute and the solvent molecules as well.

Three component ferrofluids based on D_2O were investigated at different concentration values. The results showed a strong dependence of the aggregate structure, in particular width of surfactant shells and the rate of the solvent penetration into these shells, on the concentration of ferro-particles in the fluids.

Soft materials. — The investigation of *ferrogels* on the base of chemically cross-linked PVA with attached mono-domain magnetite particles was continued. The dynamical properties of this system were studied by neutron spin-echo technique. Two kind of internal motions were observed: the first one is that of the polymer chains forming the gel, the second one is the oscillation of the magnetite particle aggregates confined in the gel network. In particular, this latter motion is characterised by the following values: the radius of the particle aggregates is R_p~9 nm, the frequency and amplitude of the oscillations are $\omega \sim 0.6 \cdot 10^{10}$ 1/s and a~1nm, respectively (at T=343 K).

An interesting feature of poly(N-vinylcaprolactam) (PVCL) that the polymer chains can form coil or globular shape aggregates in water solution. We have studied by SANS and NSE this coil-globule transition (T_C=32°C) in D_2O-solution (C=0.5wt%, mass $M=1 \cdot 10^6$). The increasing temperature enhances the interaction of the chain units and it makes the coils to be collapsed at $T \geq T_C$. Our inelastic neutron scattering experiments featured the anomalies of PVCL dynamics near the coil-globule transition: stretched oscillations of the intermediate scattering function were derived from the memory effects and chain tension relaxation by the segmental motion. In contrast to the expected dynamics of damped oscillations in collapsed coil-chains, high amplitudes of molecular motion in globules were recorded as a consequence of the breaking of water hydrogen bonds under the action of neighbouring amide groups. It means that water plays a role of a good lubricant for chain fragments in the globules, while in the coils ($T<T_C$) the water with its more regular structure lowers the chain mobility. In conclusion, our SANS and NSE data support the concept of the role of a giant water effect in the formation of glassy phase in PVCL.

Star-like poly(styrene) chains grafted to C_{60} were also studied by SANS and NSE below glass transition (T_G~94 °C). We found that in the stars the polymer chain arms are not condensed on the fullerene surfaces, but they are spread away from the C_{60}-core. We have also observed, that the interaction with the fullerene was slowing down the diffusion (β-relaxation) of chain units in the arms at T= -20 ÷70 °C (< T_G) and their relaxation time achieves 10-60 μs (an order of magnitude higher than in free PS-chains). In coexistence with these slow processes in the stars and PS we observed also a fast oscillation (periods~1ns) in the correlation function (δ-relaxation). As a result, this leads again to a dynamical model based on stretched oscillations.

Solids. — Nuclear radiation induces important changes in the microstructure of metallic components of nuclear power plant and research reactors, influencing their mechanical properties. We have carried out SANS experiments on samples of

irradiated reactor vessel material of VVER-440 type reactors and heat-treated samples of this material. In our measurements magnetic field was applied for viewing the magnetic structure effects of the materials. The difference in nanostructure between the irradiation and heat treatment case was clearly observed.

SANS studies of several diamond powders showed the fractal organization of these powders on the nano level. Under the static pressure up to 1000 MPa significant changes in the fractal network, as well as in the character of the pore surface, were observed.

As a promising field for industrial applications, we have started SANS investigations of various kind of cements. The structure of a number of cements used in reactor constructions was studied to detect the effect of different precipitates on the fractal organization of these cements. Another cement-like material group was studied. Dried sediments from the Tisza riverbank were investigated as a part of the environmental protection programme for Tisza. The fractal structure of these cements was revealed.

Fundamental research using thermal neutron scattering. — Thanks to the wave-properties of thermal neutrons various interference phenomena can be studied. Among others, we have been investigating standing waves generated as a result of interference of the incident and reflected neutron waves above a flat surface specularly reflecting from them. This standing wave carries information about the surface structure of the deposited magnetic and non-magnetic surface layer systems. Such standing waves can be observed e.g. by using nuclear reaction provided in one of the layers containing nuclei strongly absorbing neutrons. At present we have manufactured a proportional counter which serves for the registration of the nuclear reaction products appearing after the neutron-capture and in which the sample can be embedded. This counter can detect conversion electrons emitted by Gd and α-particles emitted by Li. The gas-amplification properties of the detector was measured and optimized.

Another interference effect is the observation of atomic resolution neutron holography. Since the wavelength of the thermal neutrons is comparable with the inter-atomic distance in the crystals in principle the modulation of the scattered intensity from a point-like neutrons source contains the full information of the three-dimensional arrangement of the surrounding the source atoms. This effect was demonstrated for photoelectrons and X-rays. We have carried out an estimation of the feasibility of a similar experiment using thermal neutrons. It was shown that there are several approaches for the realisation of such an experiment and the success of the experiment is not beyond the present technical limitations. These considerations were presented at international conferences and described in an article submitted for publication in Europhysics Letters, the corresponding experiments are being prepared, as well.

Developments in neutron scattering techniques. — 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 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. A new type, multibeam collimator for our SANS equipment, a new generation of velocity selectors (multiblade) are being constructed. We co-ordinate also a large-area

multiwire detector project. In the frame of the European Polarized Neutron Initiative, a polarization setup has been developed for neutron reflectometry, including Mezei- and solid state flippers as well as research is carried out on a micro-focusing polarized neutron device and a magnetic analyser. Electromagnetic field computations and design of field tailoring devices are in progress to envisage polarization and focusing of neutron beams.

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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)
HPRI-CT-1999-00099 Acces to Research Infrastructure (BNC, L. Rosta, 2000-2002)
HPRI-1999-50016-CT European Polarized Neutron Initiative (Gy. Török 2000-2002)
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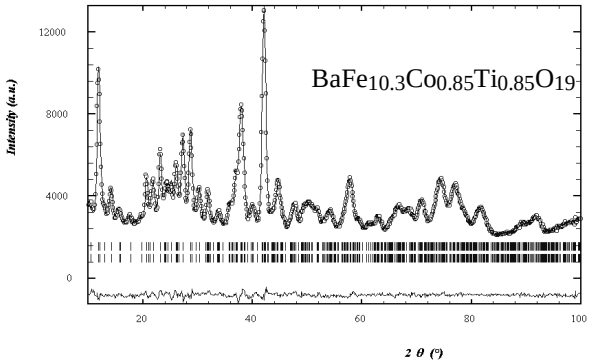
See also K.8.

K. NEUTRON SCATTERING

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

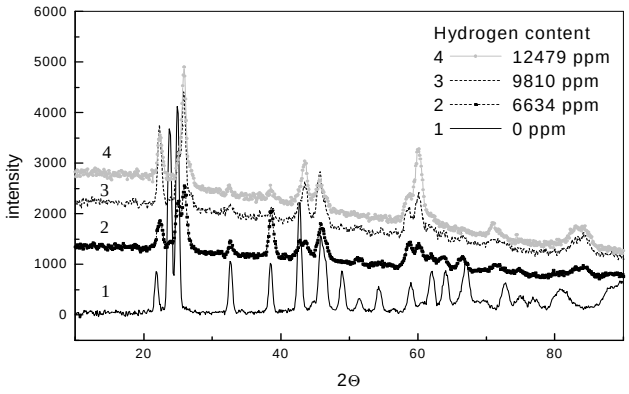
Nanocrystalline materials. — Magnetite and doped hexaferrites play important roles in many applications, i.e. in permanent magnets, or in microwave devices. These materials show new properties when prepared on a nanoscale size of particles. In order to find the correlation between magnetic properties and structural parameters, we have undertaken a systematic neutron diffraction study on several specimens with different grain size, prepared by chemical coprecipitation method. Crystalline and magnetic structure refinements were performed on **doped barium hexaferrite,** $BaFe_{10.3}Co_{0.85}Ti_{0.85}O_{19}$ samples. Crystallographic parameters were refined in space group $P6_3/mmc$ while magnetic moment values were determined in the Gorter-type ferrimagnetic arrangement. The platelet shape of the grains with a characteristic size of 14 nm along the c-axis was also determined from the observed <hkl> dependent broadening of diffraction peaks.



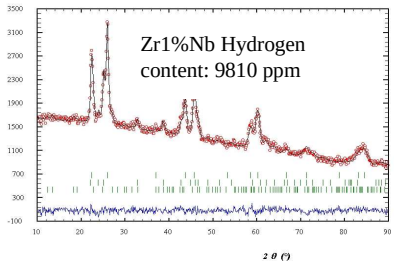
Neutron diffraction pattern and Rietveld refinement of nanocrystalline $BaFe_{10.3}Co_{0.85}Ti_{0.85}O_{19}$

Atomic structure parameters and sublattice magnetic moments for nanocrystalline **magnetite** Fe_3O_4 specimens were determined using the Rietveld refinement of neutron diffraction spectra. The sublattice magnetization at the octahedral sites of the spinel structure decreases with decreasing grain-size, while it remains practically constant at the tetrahedral sites. The existence of vacancies at the cation position is supposed.

Structural materials. — Knowledge of atomic structures of **zirconium alloys,** serving as fuel claddings, as well as of their hydrides have basic importance because the mechanical properties (e.g. embrittlement) depend on the micro- and atomic stucture. Several Zr1%Nb cladding tubes with different hydrogen content up to 13894 ppm were measured by neutron diffraction and the spectra were analysed by Rietveld method. The patterns of the pure Zr1%Nb specimens could be described well in terms of hexagonal α-Zr ($P6_3/mmc$), while the existence of other phases is evident for the hydrated samples. The transformation of α-Zr into cubic δ-ZrH_2 ($Fm3m$) with increasing hydrogen content could be observed, while a small amount of tetragonal γ-ZrH ($P4_2/n$) was also detected for each hydrated sample. The large incoherent scattering of hydrogen indicated the different hydrogen content of the samples. Large texture effects were observed influencing the Bragg intensities and leading to difficulties when performing an accurate quantitative phase analysis.



Neutron diffraction pattern of Zr1%Nb cladding tubes with increasing hydrogen content.



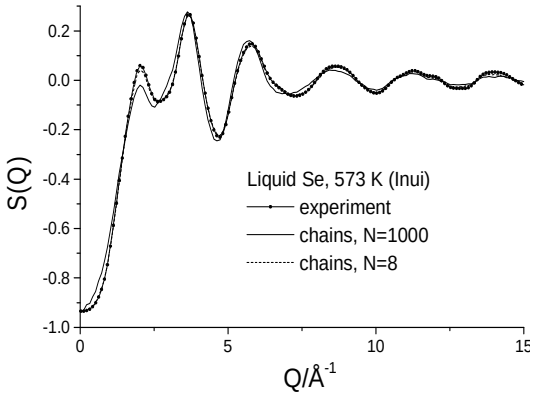
Result of the Rietveld refinement. The Bragg peak positions of the three different phases (α-Zr, δ-ZrH_2 , γ-ZrH) and the difference curve of the measured and calculated patterns are also indicated.

Temperature controller units **(**mass-produced for the industry) were tested in order to detect the origin of their defective functioning. The flow of propellant fluid in the sensor, in the capillary and in the membrane was visualized by dynamic neutron radiography. The effect of the applied technological processes on the crystalline structure of the membrane was analysed by neutron diffraction. The coexistence of ferrite (α-phase) and austenite (γ-phase) was identified in the material. As an effect of pressing, recrystallization from the FCC γ-phase to the BCC α-phase was observed that may lead to formation of internal stresses and/or dislocations, that can cause fragility of the membranes.

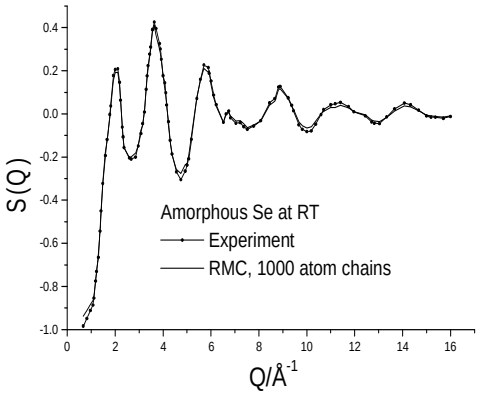
For **stress investigations** binary alloys ($Fe_{95}Cu_5$, $Cu_{95}Fe_5$, and $Cu_{95}Pb_5$) were produced. After heat treatments the existence of two-phase systems was established for each sample by neutron diffraction and by metallographic measurements. Due to the difference in the linear thermal expansion coefficients of the components, dislocations are present at the phase boundary of the matrix and of the precipitated phase leading to the development of internal strains.

Liquid and amorphous systems. **—** All accessible structural properties of **liquid water** and (high- and low-density) **amorphous ice** have been compared in detail. Based on partial structure factors and pair correlation functions and particularly, on various cosine distributions of bond angles, it is suggested that the instructive view of liquid water as a mixture of the two forms of amorphous ice is too simplistic.

Large structural models of **liquid and amorphous selenium** that were consistent with the most up-to-date X-ray and neutron diffraction results have been constructed by Reverse Monte Carlo modelling. First, the density of the amorphous phase had to be clarified: we found the value of 0.034 Å the most appropriate, which is half way between the values that had most frequently been used previously. Via the extensive use of different kinds of coordination constraints, we were able to show that already close to its melting point (around 550 K), liquid Se may form only very short chains (up to N_{max}=8), whereas close to the critical point, liquid Se can be considered as an atomic liquid (although one with a very low first coordination number). For the amorphous phase, the existence of long chains (N_{max}>1000) was found possible, as it is obvious from the Figures below. Moreover, it appears that any structural model with exactly twofold coordinated Se-atoms (e.g., 8-membered rings) may work amorphous selenium.



Structure factors of liquid Se; note that long chains are not consistent with the experiment within its errors while chains up to N=8 are.



Structure factors of amorphous Se.

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Grants:

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

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

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L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

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

Experimental studies of interactions of intense short laser pulses with metal surfaces. — Our former principle to generate strong, extreme short, attosecond duration (10^{-18} s) light pulses based on high harmonic generation has been successfully verified in the literature. To extend this principle for production of strong attosecond pulses in the X-ray range, we realized new experiments in which picosecond Neodymium-laser pulses have induced emission of strong electron pulses, ion pulses and XUV pulses of extreme wide spectra from illuminated metal cathods, in the presence of high outer electrostatic field. The obtainable very short XUV pulses are promising in high time and space resolved investigations and in different medical applications.

Theoretical study of laser – matter interaction. — 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 results concerning the generation of strong X-ray pulses at metal surfaces in the presence of a static electric field.

A new phase operator of a quantized mode of the radiation field has been constructed whose mathematical properties have been thoroughly analysed. Based on the exact solutions of the Schrödinger equation of the system consisting of an electron plus a mode of the quantized radiation field Gaussian entangled photon – electron states have been constructed. These states satisfy the number – phase minimum uncertainty relation.

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Grants

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

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L.5. G. Veres[*], J. Bakos[*], I. Földes[*], K. Gál[*], G. Kocsis[*], E. Rácz[*], S. Szatmári[*] and S. Varró: Polarization properties of harmonics generated in solid state laser plasmas. In: *"Kvantumelektronika 2000", Proc. of the 4th National Symposium on Quantum Electronics (3 November, 2000, Budapest),* Ed. S. Varró (SZFKI, Budapest 2000), P20 (in Hungarian)

M. LASER PHYSICS

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

Atmospheric pressure glow discharges. — The shape of a glow discharge operating between two copper plate electrodes was investigated in air at atmospheric pressures.

The shape of the discharge was found to depend strongly on the air pressure. The cross-section of the discharge was not constant along the discharge axis, it decreased or increased from the cathode to the anode depending on the air pressure. A relatively narrow pressure range was observed, where the discharge shape was cylindrical. This phenomenon is caused by the different pressure dependence of the cathodic and anodic current densities, which violate the similarity law because of the occurrence of dissociative recombination of molecular ions in the applied pressure ranges.

Gas laser studies. — Connected to the development of novel high-voltage heated metal-ion lasers spectroscopic measurements were carried out on different high-voltage hollow cathode discharge arrangements. The aim of the work was to find the most favorable geometry that would provide us the highest pumping rate of the laser transitions. As in most cases metal ion lasers are pumped by charge transfer reaction between noble gas ions and metal atoms. High density of both species is needed for efficient laser action. The metal vapor in heated laser tubes is produced by thermal evaporation, thus it is advantageous to suppress the sputtering of cathode material (copper in the recent experiment). We measured the intensities of He-II and Cu-I transitions that are correlated to the corresponding particle densities. Based on the results the new type ‘flat anode hollow anode-cathode’ discharge was chosen for the final applications in which high helium ion density and low concentration of copper atoms was found. Utilizing the experimental data heated zinc ion laser tube (with stainless steal cathodes) was designed, preliminary measurements are planned for the beginning of the next year.

Gas discharge research. — A self-consistent model of helium glow discharges was developed. The model is expected to be valid from low pressures up to several hundred millibars. The aim of these studies was to observe how the molecular helium ions become important in the discharge at higher pressures and to identify the important source and loss processes of atomic and molecular ions at different pressures. We have also carried out an experiment and recorded the voltage-current characteristics, as well as light emission spectra (including helium molecular bands) of the discharge at different pressures and different separations of a plane-parallel electrodes.

Research on multidimensional lasers. — In order to simulate naturally occurring laser materials, such as living organelles, having randomly distributed highly scattering and emitting microstructures, a non classical, point-source like three-dimensional random interference pattern (RIP) micro-laser ensemble emission was realized by coherent random interference pattern excitation. The results of our experiments enabled us to distinguish the observed new phenomenon from the classical amplified spontaneous emission. The mostly thresholdless appearance of laser emission indicates the operation of independent microlasers. In microlasers which occur in nature we expect to find a completely analogous process, whereas in

nature precisely adjusted laser mirrors are hardly found, biological specimens often possess coarse structure.

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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 modelling of gas discharge plasmas (Z. Donkó, 1998-2001)
OTKA F-25503	Hollow cathode discharges and lasers in gold vapour (G. Bánó, 1998-2001)
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N. FEMTOSECOND LASERS

R. Szipőcs, P. Apai, S. Lakó

Optical thin-films in femtosecond laser systems. — Continuing our research started in 1993, dispersive dielectric mirrors were developed for different femtosecond laser systems such as: (a) 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 optimization 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 Philipps 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. — 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.

Second-harmonic generation. — A synchronously pumped, mirror-dispersion-controlled ring oscillator has been built in our laboratory for high efficiency second-harmonic generation of broadband femtosecond laser pulses delivered by a mirror-dispersion controlled Ti:sapphire laser. We observed a 800% increase in the conversion efficiency relative to the single pass conversion when the cavity length was adjusted to fit the repetition rate of laser.

Continuum generation. — In collaboration with Bell Laboratory of Lucent Technologies Inc. (USA), and researchers from PTE[+] (Pécs, Hungary) and SzTE[++] (Szeged, Hungary), femtosecond pulse white light continuum was generated in

[+] PTE=University of Pécs

[++] SZTE=University of Szeged

microstructure optical fibers using 1-10 nJ, 80..150 fs pulses from our tunable Ti:sapphire laser. We investigated spectral intensity and phase of the continuum as the function of laser parameters (energy, central wavelength, chirp and bandwidth of the laser pulse) and as the function of fiber length. We found that the continuum slightly chirped when exiting the fiber: we measured an interferometric autocorrelation trace corresponding to a 19 fs pulse when the spectrum corresponded to approximately 9 fs transform limited pulses.

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Grants

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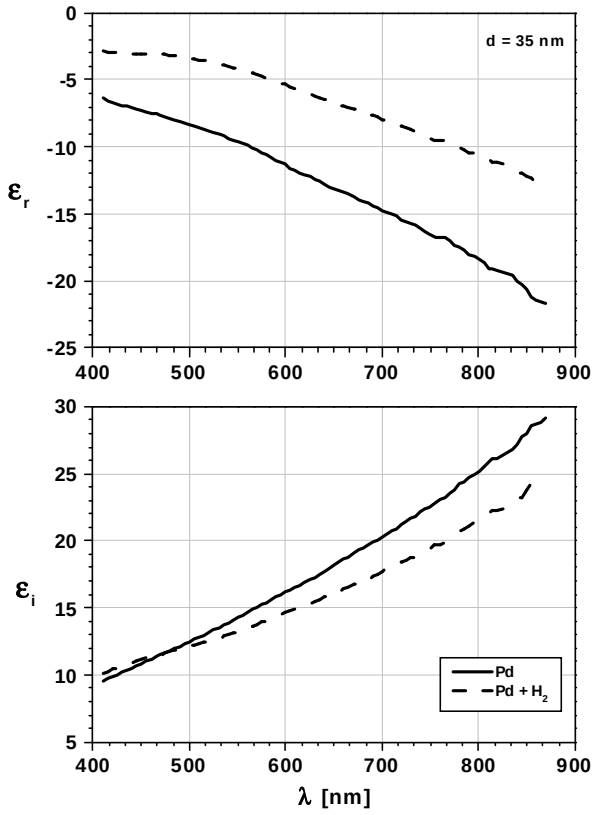
O. METAL OPTICS

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

Optical investigation of fullerene films. — A high vacuum ($5 \cdot 10^{-4}$ Pa) source was constructed for C_{60} sublimation. Thin films of 36-620 nm thickness were prepared with condensation rates between 0.8-5.1 Å/s on room temperature (40 °C) and heated (140 °C) BK-7 glass substrates. The complex optical dielectric function of fullerene films were determined with an optical multichannel analyser (OMA-4) based attenuated total reflection (ATR) reflectometer in the 400-850 nm wavelength range at room temperature and laboratory environments. Simultaneously, surface morphology of the samples (average rms roughness amplitude and grain size) was determined with an atomic force (AFM) microscope. It was found that slowly evaporated, evaporated onto hot substrate, or normally evaporated and post-annealed films show very high rms roughness amplitudes (up to 43 nm). The enhanced roughness had drastic influence on the optical behavior of fullerene layers. The shift of ε_r and ε_i can not be explained by scalar theories.

Optical behavior of hydrogenated Pd films. — Pd films of 35 nm thickness were evaporated on BK-7 glass substrates in $7 \cdot 10^{-4}$ Pa pressure with 5 Å/s rate. In the first time, we determinated the change of its complex dielectric function under the influence of dry, 4N pure hydrogen gas of 1 bar pressure with our ATR reflectometer. The absolute value of both ε_r and ε_i decreased in hydrogenated samples, where 0.7



Changes in the complex dielectric function of a 35 nm thich Pd film under the influence of 4N pure hydrogen gas of 1 bar pressure.

H/Pd atomic ratio is expected. This change was reversible. DC electric resistivity was also determined, and reversibly increasing film resistivities were found in H_2 atmosphere. Evaluation of the dielectric function of samples resulted in a decreasing plasmon energy (6.29→5.25 eV) and decreasing relative specific density of electrons of conductivity (1→0.7).

Thermoluminescent (TL) emission spectra. — An OMA-4 based, multichannel spectrometer was constructed with photon-counting sensitivity for determination of emission spectra of TL materials in the wavelength range 380-850 nm. The setup was tested with 0.6-1.2 Gy β-irradiated, polycrystalline Al_2O_3:C tablets. Heating rate was 5°C/s, maximum temperature 300°C, exposition time 2 s. 30 spectra were taken during 1 min of linear heating cycle. It was found that the carbon doped aluminium oxide has two emission bands at 420 and 520 nm, which show maximums at 191 and 217°C, respectively. No emission was found above 650 nm.

Near-field optical study of grainy noble metal films. — Surface plasmons were excited using the ATR technique with a Kr laser in thin films of Ag and Au, having small islands from Au and Ag, respectively. Emission of plasmon-induced light was studied with a scanning tunneling microscope (STM) using W or Au tips. It was found that the quality of the STM picture (resolution and contrast) is much better when tips and layers were made of materials of different chemical potential.

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Grants

OTKA T-020089	Optical parameters of fullerene films (Z. Szentirmay, 1996-2000)
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P. LASER APPLICATION

A. Czitrovszky, P. Jani, I. Kertész, Á. Kiss, M. Koós, A. Nagy, I. Pócsik, J. Tóth, M. Veres

Optical measuring techniques. — A new quantum optical measuring system based on the generation of entangled photons was developed for standardless calibration of the linear photon counting detectors at different operating conditions. Using the developed units - time-to pulse height converters and multichannel analyzers in the investigation of photon statistics, a 2ps/channel resolution was achieved. A series of different photomultipliers were measured and selected for future experiments.

A new measuring head for an airborne particle counter was developed with increased sensitivity, better signal/noise ratio and improved signal evaluation system. This measuring head will be installed in the new particle counter which is under development for measurement of aerosols released from LWR fuel rods at 2000^{o}C in a large-scale nuclear accident simulation experiment in the frame of EU COLOSS program.

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

A modelling of a forward-backward scattering airborne particle counter was performed in collaboration with the Vienna University. The scattering geometry, illumination and detection conditions, appropriate data evaluation parameters were determined. A new measuring unit for such device was designed, constructed and tested. The system has a number of benefits in comparison with the previous airborne particle counters.

Work in the field of integrated optical sensors for the revelation of laser radiation, its presence and direction of propagation has been started.

Solid state laser development. — The development and application of Er:glass laser was continued. The optimization of the cooling system was performed and increasing the repetition rate was achieved.

In collaboration with GE LIGHTING Co., a cutting technology for combined W-Mo coils was developed using a laser system based on a Nd:YAG laser. This technology was optimized for different cutting conditions.

Amorphous thin layers. — A new technology was developed to prepare amorphous carbon nano-particles. The speciality of this material is its non-graphitic character, which of course can be induced by further thermal annealing. This material has large potential for practical application, like using it for the large surface super-capacitor. This material can be prepared under different conditions, so its structure, physical and chemical properties can be varied. The morphological investigations showed nice spherical shape of these particles in the 10-100 nm diameter range. These particles aggregate into low-dimensional structures. Bonding properties of carbon and hydrogen atoms studied by infrared measurements show the presence of sp^1, sp^2 and sp^3 hybridised carbon sites. The electronic structure exhibits optical gap not smaller than ~2eV, as it was determined from the photoluminescence excitation spectra. Effective light emission at room temperature of these particles have also been observed, when it was excited by optical photons.

The photoluminescence (PL) study of amorphous carbon (a-C:H) thin layers was continued with the aim to understand the origin of light emission and the recombination mechanism. We have investigated the broadening of the visible photoluminescence spectra of a-C:H layers at different excitation photon energies. The wide PL spectra become asymmetric as the exciting photons are in the emission band. This experimental result proves that the broadening of PL spectrum is inhomogeneous; it consists of several homogeneously broadened bands. This behaviour can be related to the distribution of electronic levels through which radiative recombination takes pace. We have investigated the ultraviolet (UV) luminescence, observed by us earlier on samples prepared at different conditions to find correlation between UV light emission and structural properties of the layers. From the absorption measurements in the UV and visible region we have determined the optical forbidden gaps of these samples. The comparison of these data with the results of infrared study we can make a conclusion that a small structural unit (3-6 Å) with conjugated double bonds, either in olefin or in aromatic local configuration, can be responsible for UV light emission.

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Grants

EURATOM COLOSS (5th. Framework), project FIKS –CT 1999-00002 subcontract, CODEX B4C experiment (A. Czitrovszky, 2000-2001)

OMFB Contract No 00887/99 Development of the DMA for the detemination of the electrical charge of nuclear aerosol particles (A. Czitrovszky, 1999-2001)

OMFB Contract No 02126/99 Integrated optical sensor for the revelation of laser radiation, its presence and direction of propagation (P. Jani 1999-2001)

GE – SZFKI No 472/2000 Development of cutting technology for W-Mo coils (I. Kertész, 2000)

Austro-Hungarian Bilateral Contract No A24/2000, Development of dual wavelength particle counter (A. Czitrovszky, 2000-2001)

OTKA T-026073 Electronic states, charge carrier localization and their interaction with the structure in amorphous carbon films (M. Koós, 1998-2000)

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Q. OPTICAL THIN FILMS

K. Ferencz

Optical thin film structures in femtosecond laser systems. — Our research was continued in development of dispersive dielectric mirrors for different femtosecond laser systems such as low-loss chirped mirrors for mode-locked Cr:LiSGaF, Cr:LiSAF lasers, for broadly tunable cw, modelocked Ti:sapphire lasers, 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 were developed for these applications.

Other developments on optical coatings. — Our work on optical waveguides deposited on optical gratings is still in progress for optical sensors used for medical applications. We started basic experiments in nanobiological application of optical waveguides. 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.

Special interference filters were developed for high sensitivity detection of protein molecules elaborated by gene manipulation methods.

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Grants:

OPTILAB - SZFKI No 364 Nanobiologycal application of optical thin films (Kárpát Ferencz, 2000)

R. 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. — New characterization methods were developed and applied for the non-linear β-BaB_2O_4 (BBO) crystals. The effective non-linearity, d_{eff} for type I and type II phase matched BBO crystals were determined by a room temperature absolute measurement with an accuracy better than 10%. The frequency conversion efficiency was measured as function of the deviation from the phase-matching direction. The angular bandwidths from these experiments were modeled and interpreted.

A modified Michelson interferometric technique was applied to determine all components of the electro-optic (EO) tensor in BBO. With this technique, high accuracy can be achieved even with small values of the EO coefficients. The relative sign of EO coefficients, the change of the sample dimensions due to the piezoelectric effect, and the influence of the temperature are also considered.

The thermal parameters of the individual crystal phases were determined in the Y_2O_3—B_2O_3—Al_2O_3 system and its subsystems. The YBO_3 formation in the Y_2O_3—B_2O_3 subsystem is accompanied by exothermic heat effects in the 700 – 1000 ^oC range. Exothermic formation of $Al_4B_2O_9$ has been observed in the 900 – 1000 ^OC range in the B_2O_3—Al_2O_3 subsystem. This compound decomposes to $Al_{18}B_4O_{33}$ and B_2O_3 between 1050 and 1150 ^oC. Both the basic oxide mixtures and the two intermediers from the subsystems produce the required starting material of $YAl_3(BO_3)_4$ (YAB) for the crystal growth. above 1150 ^oC.

Growth and study of stoichiometric lithium niobate crystals. — The effect of growth conditions was investigated on the crystal perfection of stoichiometric lithium niobate $LiNbO_3$ prepared by the high temperature top seeded solution growth technique (HTTSSG) from K-containing flux. Flux compositions between 0.09-0.21 $K_2O/LiNbO_3$ ratio were tested, and it was found that $LiNbO_3$ forms a eutectic system with the K_2O (close to the 1:5 molar ratio of K_2O and $LiNbO_3$). This composition is considered as the solvent in the system. Stoichiometric crystals with homogeneous composition were grown from fluxes in the range of 0.16-0.195 $K_2O/LiNbO_3$ ratio. The formation of the structural defects have been examined for different growth directions. Facet developments occurred primary along the {01.2} pyramidal planes. Close connection was found between faceted growth and the appearance of domain reversal.

Electric field induced periodic poling of 3 mm thick stoichiometric lithium niobate was first reported. The suitable poling field (200 V/mm) was 2 orders of magnitude lower than in the congruent material, and 20 times lower than in previously published results on near-stoichiometric crystals.

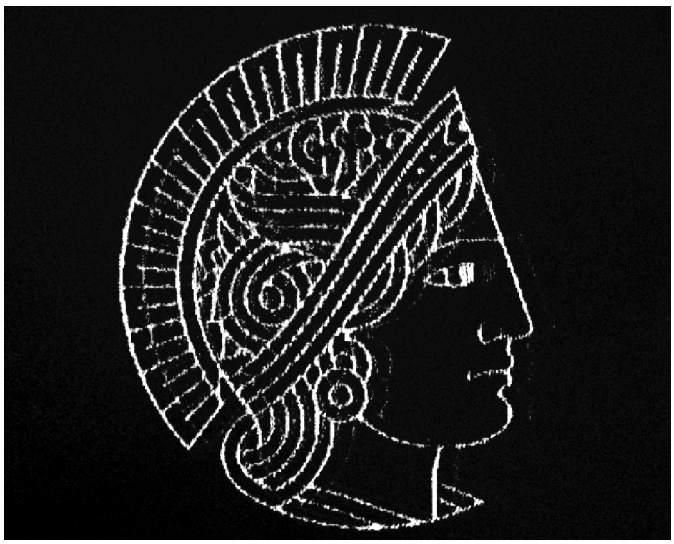
Comparative studies of congruent and near stoichiometric $LiNbO_3$ single crystals using hyperfine interaction and ion-beam techniques show that the structure of the congruent $LiNbO_3$ cannot be completely described by the models assuming only Li vacancies and Nb anti-sites. The additional defects are cation stacking inversions in which the cation sequence coincides locally with an ilmenite-like $LiNbO_3$.

The lattice-site location of Co ions has been determined in congruent $LiNbO_3$ doped with Co by particle-induced X-ray emission combined with channeling techniques. Co has been found to occupy exclusively Li site.

Growth and study of bismuth tellurite crystals. — Single crystals of pure and Er doped Bi_2TeO_5 were grown by the Czochralski technique.

The dependence of the four-wave mixing diffraction efficiency on the crystal orientation, incident beam polarization and grating vector direction was analyzed. Applying 532 nm write beams of a cw Nd:YAG laser, **the saturation diffraction efficiency was above 40%** in the optimum configuration (G|| [100], P||[001]) which is competitive to the best photorefractive crystals. The stability of the written grating under strong erase beam was better than that of the reference $LiNbO_3$ samples. Using 13 W/cm^2 erase intensity for 8 minutes, the Bi_2TeO_5 crystals conserved 11 % of the starting diffraction efficiency while the $LiNbO_3$ only 0.3 %.

The first two-dimensional analog hologram was written in Bi_2TeO_5 crystals (see figure).



The energy levels of the crystal field transitions and their Stark components were determined for Er^{3+} ions in Bi_2TeO_5. The temperature dependence of the occupation of the non-zero Stark levels was analyzed. It was shown that the Er^{3+} ions occupy the different Bi-sites in the crystal, which represent perturbed cubes of 8 and 7 oxygens.

Analytical spectroscopic investigation of oxide crystals. — Multi-element graphite furnace atomic absorption spectrometry (GFAAS) methods are developed and studied for the simultaneous determination of Cr, Mo, and V dopants in bismuth tellurite single crystals. Since the bismuth tellurite matrix can be almost completely evaporated in the graphite furnace at the optimal pre-treatment temperature, with a multiple dosing and pre-concentration method a higher sensitivity is attained for the determinations.

A novel method based on halogenation is developed for the elimination of the memory effects, which occurs during the GFAAS determination of heavily volatilized sample components such as Er, Nd dopants in the refractory $LiNbO_3$ crystals. Carbon tetrachloride was introduced into the graphite furnace, and used with

an optimized clean-out program. By this technique, a complete removal of the sample constituents was accomplished.

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Grants

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, 1997-2000)

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)

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

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

COST Action P2 Application of nonlinear optical phenomena:
Project WG1/1. Materials and systems for optical data storage (I. Földvári, 1998-2001)
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See also: K.7., S.1., S.3., S.8., S.10., S.11.

S. CHARACTERIZATION AND POINT DEFECT STUDIES OF OPTICAL CRYSTALS

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

Characterization of optical crystals. — A systematic study of the electrical conductivity of Bi_2TeO_5 single crystals has been carried out within a wide range of temperature and in different ambient atmospheres using impedance spectroscopy and dc measurement. The single crystals are found to be mixed conductors in which electronic conduction and ionic conduction coexist. The conductivity of the crystals along the [100] direction is much smaller than in directions perpendicular to it. The ambient atmosphere effects the electrical conductivity. The Cr-doping increases the conductivity in the [001] and [010] directions.

Microscopy of crystal imperfections. — Using optical and electron microscopic methods the as-grown surface and inner microstructure of numerous $YAl_3(BO_3)_4$ (YAB) single crystals grown from undoped and doped high temperature melt solutions have been inspected. Some minority impurity elements, such as Ca, Si and Ti were found by electron beam microanalysis which may also play a role in the formation of as-grown microdefects of YAB, besides the flux and dopant elements established earlier.

Point defects in $ZnWO_4$ and other oxide crystals. — In the scintillator $ZnWO_4$ most of the known centres are impurity related. In $ZnWO_4$ X-irradiated at ~15 K, an intrinsic O^- centre has been identified by Electron Spin Resonance (ESR) and Electron Nuclear Double Resonance (ENDOR) spectroscopy with principal g values typical for this type of centres. Super hyperfine (SHF) interactions with host cations like three W (two stronger and one weeker interactions) and one Zn ions give information about the geometry of the O^- ion: the hole resides at an oxygen which has two nearest W and one Zn rather than at the other O which has two Zn and one W as nearest neighbour ions. The defect becomes thermally unstable above 75 K. The present O^- centre is an intrinsic defect because of its low stability and the lack of any impurity related SHF interaction in its ESR spectrum. Above 23 K broadening of the ESR lines and averaging of the g values are observed which is explained by thermally activated hopping of the hole between energetically equivalent oxygen positions. The activation energy of this reorientation is found to be 16 ± 3 MeV.

Infrared spectroscopy of hydroxyl ions in oxide crystals. — The spectroscopic properties of hydrogen bound to a large variety of synthetic compounds like simple oxides, perovskites, the $LiNbO_3$ family, kalium thyonil phosphate (KTP), sillenites, eulytites, borates, garnets, spinels etc. have been reviewed using our own and literature data. In almost all compounds the OH-stretch mode was found in the range 3200—3700 cm^{-1}, with isotope replica of deuterium (2350—2750 cm^{-1}) and a few examples of tritium (2050—2250 cm^{-1}). The fundamental vibration, the isotope replica and the corresponding overtones were described with an anharmonic oscillator model. A nonlinear relation between the anharmonicity and the harmonic frequency was found and interpreted using recent second order perturbation calculations. An often pronounced temperature dependence of the stretch mode and phonon coupling was discussed. Data for the stretching vibration influenced by additional weak or strong doping were presented. Atomistic defect models were also

described and tested by means of light polarization, external perturbations like pressure and electric field, and Raman scattering analyzed with the behavior-type method.

Kinetics of the complex OH^- stretching vibrational band has been studied in a nearly stoichiometric $LiNbO_3$ crystal (Li/Nb ≈ 0.99) between 40-120 °C. The intensity of the absorption band components at a given temperature changes with time suggesting that protons migrate among different sites until they reach a thermodynamic equilibrium. The exponential time constants and the corresponding activation energies ($E_{av} \approx 1.1 \pm 0.1$ eV) were determined and compared with those of the thermal fixing process. The results obtained confirm that the hologram fixing process is governed by proton migration in the crystal.

Investigation of point defects in $LiNbO_3$ single crystals. — Transient optical absorption and luminescence induced by ionising radiation has been observed in congruent, stoichiometric, and Mg-doped $LiNbO_3$. A short-lived infrared absorption band near 1.0 eV can be attributed to intrinsic Nb^{4+} small electron polarons moving via hopping motion, the process leading at low temperatures to trapping mainly at Nb_{Li} antisite defects (absent in Mg-doped $LiNbO_3$) or to recombination with hole-type polarons. As shown by comparison with similar results in $KNbO_3$, polaron formation and recombination processes occur within niobium-oxygen complexes and are only slightly affected by alkali ions. Er doped $LiNbO_3$ crystals used for waveguide production were investigated by ESR and optically detected paramagnetic resonance (ODMR) showing various slightly different incorporation sites of the dopant. These were also characterised by detailed optical absorption and emission measurements taken also in high magnetic fields leading to Zeeman shifts and splittings of the optical transitions.

Investigation of X-ray storage phosphors. — ODMR and ESR studies were carried out in Eu^{2+} doped BaFBr single crystals and fluorobromozirconate glass ceramics to characterize the charge transfer and optical excitation processes underlying X-ray imaging applications of these materials. An ESR investigation of Eu^{2+} doped $BaBr_2$ single crystals and powders showed that Eu^{2+} substitutes for Ba^{2+} and has the same ESR parameters in $BaBr_2$ than in the fluorobromozirconate glass ceramics. This proves that the X-ray storage phosphor properties of the investigated ceramic system can be attributed to $BaBr_2$:Eu^{2+} inclusions.

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Grants

OTKA T 022859 Determination of the structure of point defects by spectroscopic, conductivity and quantum chemical methods. (A. Watterich, 1997-2001)

OTKA T 023092 Characterization of multicomponent nonlinear optical crystals. (E. Hartmann, 1997-2001)

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

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See also R. 15, R. 16, R. 21, R. 22 and K.7

T. NONLINEAR AND QUANTUM OPTICS

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

Laser-induced molecular dynamics. — Resonant driving of certain electronic transitions in diatomic molecules is shown to yield collapses and revivals of the electronic populations due to the quantized vibrational motion of the nuclei. In contrast to the usual Jaynes-Cummins model here the electromagnetic field is not quantized. We analyzed the properties of the vibrational potentials, the frequency and power of the classical driving laser field for which this effect can be observed. We have shown that the nonlinearity of the potential may lead to a more pronounced effect and we have found the reason for it.

Nonlocal quantum states and quantum teleportation. — We have investigated the classical analogue of quantum teleportation: we have examined what happens to Bennett's teleportation scheme, when the density matrix elements of the Einstein-Podolsky-Rosen pair, which are off-diagonal on product basis, are reduced. By setting these to zero, we have obtained the classical one-time pad cypher, as a classical limit of quantum teleportation. The reduction of the matrix elements by a nonzero factor provides an interpolation between the classical and quantum cases. We have demonstrated the reduction of the teleportation fidelity on the behavior of statistics and fidelity of a gedankenexperiment.

We have applied the correspondence between conjugate linear maps and entangled states for the classification of all finite dimensional Bennett type teleportation schemes applying pure states. We have obtained a necessary and sufficient condition of teleportation and state truncation for the entangled state and the joint measurement involved in the scheme. The formulation of the condition does not require a choice of a basis on the Hilbert-spaces.

Nonlinear optical processes. — A general method is developed for analysing the evolution of nonclassical light in complex two-mode optical systems where linear and nonlinear processes with quadratic Hamiltonians can take place simultaneously or successively. Analytic expressions are derived for the output Wigner function and the output photon number distribution for a general coherent-state superposition input that can approximate any quantum state of light with a high degree of accuracy. As an example, the evolution of amplitude squeezed light is analysed in a nonlinear coupler with degenerate and nondegenerate parametric amplification. It is shown that all-optical switching can be realized in this system.

Cavity quantum electrodynamics and microlasers. — We proposed a new method for detecting and monitoring the motion of a single atom in high Q optical resonators based on the position sensitive dispersive coupling of different field modes. Using sufficient atom-field detuning the irreversible evolution of the internal state and external motion of the atom can be kept small still allowing for a fast and reliable detection. As an implementation we discussed the case of two counterpropagating modes in a microscopic ring resonator with spatially localized output coupler. The analytical estimates yielding 100% signal contrast for suitable parameters are then confirmed by numerical solution of the time dependent equations for the coupled atom-cavity dynamics.

We showed that an ensemble of optically polarizable particles moving in the field of a high Q multimode optical cavity can be cooled via the correlated dynamics of the field and the particles motion. Using a large detuning between the field and the atoms, spontaneous emission plays a negligible role in this dynamics. For the special case of a two mode ring cavity and assuming small deviations of the particles from the potential minima, we found a rapid damping of the center-of-mass motion and slow damping for the relative oscillations.

Trapped atoms. — The preparation of dark nonlinear angular momentum eigenstates of the motion of a trapped ion was considered. These states are entangled states, hence they could be interesting in many applications. In our scheme a dipole allowed transition of an ion is driven by running wave laser fields. Two laser fields realize the angular momentum Hamiltonian, while a third one sets an eigenvalue. It is shown that pure angular momentum states cannot be obtained as dark states due to the degenerate eigenvalue spectrum of the angular momentum operators. Instead, the degeneracy of the eigenvalue spectrum can be removed by taking into account the nonlinearities arising from the non-vanishing Lamb-Dicke parameter associated with the laser-ion interaction. A further feature of the scheme that it leads to a dark state which is roboust against some decoherence effects as it was demonstrated numerically using quantum trajectory simulations.

Nuclear motion in molecules. — Correlation has been observed between the experimentally determined harmonic frequencies and anharmonicity coefficients of OH bond stretching vibrations in alkali halide, oxide, and hydrate crystals. We have shown that simple second order perturbation approximation formulas can account for the observed correlation and they can be used to obtain the shape of the stretching potential and an estimate of the equilibrium length of an OH bond in crystalline environment. We have investigated the relationship between the so called reconstruction method and a Baysian approach to construct potential energy surfaces of molecules. We have studied if the filter diagonalization method could be used to resolve overlapping IR bands often encountered in solid state IR spectroscopy.

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Grants:

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)

OTKA F 032341	Light-matter interaction in complex quantum systems (P. Domokos, 2000-2002)
OTKA F 032346	State reconstruction and preparation in quantum-optical systems (T. Kiss, 2000-2002)

Publications:

Articles

T.1. P. Domokos, T. Kiss, J. Janszky, A. Zucchetti*, Z. Kis, and W. Vogel*: Collapse and revival in laser-driven diatomic molecules. *Chem. Phys. Lett.* **322**, 255-262 (2000).

T.2. M. Koniorczyk, Z. Kurucz, A. Gábris and J. Janszky: General optical state truncation and its teleportation. *Phys. Rev. A* **62**, 013802 (2000).

T.3. Z. Kis, T. Kiss, J. Janszky, P. Adam, S. Wallentowitz*, and W. Vogel*: Detection of nonclassical oscillations in phase space by cascaded optical homodyning. *Laser Physics* **10**, 90-92 (2000).

T.4. P. Domokos, J. Hare*, V. Lefèvre*, J. M. Raimond*, S. Haroche*, I. Protsenko*, and L. Davidovich*: Quantum theory of microlasers in the close-to-threshold regime. *Laser Physics* **10**, 42-47 (2000).

T.5. A. Karpati, P. Adam, J. Janszky, M. Bertolotti*, and C. Sibilia*: Non-classical light in complex optical systems. *J. Opt. B*, **2**, 133-139 (2000).

T.6. P. Adam, A. Karpati, J. Janszky, S. Szabo, and E. Lugosi*: Relations between Input and Output Quantum States of Integrated Optical Systems. *Laser Physics* **10**, 127-132 (2000).

T.7. S. Szabo, P. Adam, and J. Janszky: Phase Optimized States via Coherent-State Superpositions. *Laser Physics* **10**, 139-142 (2000).

T.8. P. Domokos, M. Gangl*, and H. Ritsch*: Single atom detection in high-Q multimode cavities. *Opt. Commun.*, accepted for publication.

T.9. M. Gangl*, P. Horak*, P. Domokos, and H. Ritsch*: Collective cooling of neutral particles in cavities without spontaneous emission. *Laser Physics*, accepted for publication.

Others

T.10. Janszky J., Szabó G.*: Laser physics and modern optics. In: *Physical Science at the Millennium*, Ed. Nagy K., MTA, Budapest, 2000, pp. 47-58. (in Hungarian)

T.11. Janszky J.: In memoriam Tarján Imre, *Magyar Tudomány* 2000/9, pp. 1157-1159.

EDUCATION

Graduate and postgraduate courses, 2000

— Completely integrable many body systems, (F. Woynarovich, ELTE[3])

— Solid State Physics (J. Sólyom, ELTE)

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

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

— Thermodynamics and statistical physics (F. Iglói, SZTE)

— Surface Magnetism (B. Újfalussy, ELTE)

— Electron Correlation and Magnetism I. (P. Fazekas, BME[5])

— Electron Correlation and Magnetism II. (P. Fazekas, BME)

— Advanced Solid State Physics III. (I. Tüttő, ELTE)

— Optical Properties of Solid State (I. Tüttő, ELTE)

— Electronic States in Solids (J. Kollár, ELTE)

— Metal Physics (J. Kollár, BME)

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

— Amorphous and crystalline materials (P. Deák*, S. Kugler* and T. Kemény, BME)

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

— Macromolecules (S. Pekker, ELTE)

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

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

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

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

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

— Liquid crystals as matrix materials for display devices (K. Fodor-Csorba, ELTE)

— Nanophase metals: Magnetism and electrical transport (I. Bakonyi, ELTE)

— Nanophase metals (I. Bakonyi, Tokyo Metropolitan University)

— Advanced material technology (G. Konczos, BME and ELTE)

— NMR spectroscopy (K. Tompa, BME)

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

— Neutron scattering in condensed matter (L. Cser, ELTE)

[3] ELTE= Loránd Eötvös University, Budapest

[4] SZTE= University of Szeged

[5] BME= Budapest University of Technology and Economics

— Computing in chemistry (L. Pusztai, ELTE)

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

— Applied Quantum Electrodynamics (S. Varró, PTE[6])

— Selected Problems in Quantum Optics and Strong Field Electrodynamics (S. Varró, SZTE)

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

— Physics of Amorphous Matter I. (M. Koós and I. Pócsik, SZTE)

— Physics of Amorphous Matter II. (I. Pócsik and M. Koós, SZTE)

— Crystal Physics of Optical Materials (I. Földvári, Á. Péter, BME)

— Crystal Growth from the Melt (in: Crystalline and Amorphous Materials, K. Polgár, BME)

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

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

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

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

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

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

— Statistical quantum optics I (J. Janszky ELTE)

— Statistical quantum optics II (J. Janszky, T. Kiss, ELTE)

— Thermodynamics and statistical physics (T. Kiss, PTE)

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

— Numerical physics (P. Ádám, M. Koniorczyk, PTE)

Laboratory practice and seminars

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

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

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

— Basic experimental physics (L. Gránásy, BME)

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

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

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

— Superconductivity seminar (G. Kriza, BME)

[6] PTE=University of Pécs

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

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

— Neutron scattering (L. Rosta, BME)

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

— Neutron scattering in material research (L. Rosta, ME[7])

— Neutron detectors (E. Rétfalvi, BME)

— International graduate training in neutron scattering (L. Cser, Gy. Török, M. Avdeev, Hungarian-Austrian Fund)

— Medical application of lasers (Z. Gy. Horváth; SOTE[8], Medical Laser Center)

— Seminars on biophysics for medical students (K. Szőcs, SOTE).

— Measurements in holography and metal optics (Z. Szentirmay, ELTE)

— Theoretical physics, seminar (P. Ádám, PTE)

— Thermodynamics and statistical physics (T. Kiss, PTE)

— Quantum mechanics (M. Koniorczyk, PTE)

— Quantum mechanics (A. Kárpáti, PTE)

— Elementary calculus and linear algebra (M. Koniorczyk, PTE)

Diploma works

— L. Németh (ELTE): ^{77}Se NMR spectrum and spin-lattice relaxation in the charge-density wave phase of $(TaSe_4)_2I$ (Consultant: G. Kriza)
K. Lengyel (ELTE): Thermally fixed holograms and absorption of OH^- ions in nearly stoichiometric $LiNbO_3$ crystal (Supervisor: L. Kovács)

— A. Kárpáti (ELTE): Nonclassical states in complex optical systems (Supervisor: P. Ádám)

— E. Furka (PTE): Numerical methods to solve the Schrödinger equation (Supervisor: Zs. Kis)

Ph. D. students

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

E. Benkler (Darmstadt University of Technology): Photoinduced modification of intermolecular interactions and optically controlled materials. (Hungarian coadvisor: I. Jánossy)

[7] ME=University of Miskolc

[8] SOTE=Semmelweis Medical University, Budapest

E. Szabó (ELTE): Synthesis and properties of banana shaped liquid crystals (Supervisor: K. Fodor-Csorba)

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

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

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

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

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 liquid mixtures by neutron scattering (Supervisor: L. Cser)

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

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

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

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

K. Mocsár (BME): Production of superintense, ultrashort laser pulses and investigation and interpretation of the new type nonlinear interactions of laser light and matter (Supervisor: Gy. Farkas)

G. Bánó (SZTE): Metal-ion lasers (Supervisor: K. Rózsa)

P. Horváth (ELTE): Metal-ion lasers (Supervisor: K. Rózsa)

P. Hartmann (ELTE): Elementary processes in gas discharges (Supervisor: Z. Donkó)

K. Kutasi (PTE): Elementary processes in gas discharges (Supervisor: Z. Donkó)

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

S. Lakó (SZTE): Nonlinear frequency conversion of femtosecond laser pulses (Supervisor: R. Szipőcs)

A. Nagy (ELTE): Investigation of the optical properies of airborne particles (Supervisor A. Czitrovszky)

Z. Lipp (BME): Laser Doppler velocimetry (Supervisor P. Jani)

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

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

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

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

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

Dissertations

M. Tegze: X-ray holography (D.Sc., Hungarian Academy of Sciences)

L. Pusztai: Inverse methods for the evaluation and interpretation of (liquid and amorphous) diffraction data (D.Sc., Hungarian Academy of Sciences)

G. Palágyi: Phase transitions in inhomogeneous and dilute spin models. (Ph.D., ELTE)

M. Bokor: NMR relaxation in Fe and Zn ionic crystals (Ph.D., ELTE)

P. Jóvári: Neutron diffraction and computer simulation studies of molecular liquids (Ph.D., ELTE)

L. Bencs: Study on graphite furnace atomic absorption methods for the determination of dopants in bismuth tellurite optical single crystals (Ph.D., ELTE).

P. Domokos: Cavity quantum electrodynamics (PhD, ELTE)

Z. Kis: Nonclassical vibrational states (PhD, JATE)

AWARDS

— G. Fáth, Bolyai Grant (1999-2002)

— Ö. Legeza, Bolyai Grant (2000-2003)

— K. Penc, Bolyai Grant (1999-2002)

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

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

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

— I. Iglói, Széchényi Professorship (1997-2000)

— D. Kaptás, Bolyai grant (1999-2002)

— L. Gránásy, Physics Award of the Hungarian Academy of Sciences (2000)

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

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

— G. Oszlányi, Bolyai Grant (1998-2001)

— T. Börzsönyi, Publication Award of the Research Institute for Solid State Physics and Optics (2000)

— Á. Buka, Széchenyi Professorship (1998-2001)

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

— M. Bokor, Young Scientist's Award of the Hungarian Academy of Sciences (2000)

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

— Gy. Farkas, Principal Award of Physics of the Hungarian Academy of Sciences (2000)

— Z. Donkó, Bolyai Grant (1998-2001)

— R. Szipőcs, Bolyai Grant (1999-2001)

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

— L. Kovács, Z. Gyulai Award, Roland Eötvös Physical Society (1999)

— J. Janszky, Széchenyi Professorship (1998-2001)

— P. Ádám, Széchenyi Professorship (1997-2000)

— T. Kiss, Bolyai Grant (1999-2001)

CONFERENCE

— 7th Central European Workshop on Quantum Optics, Balatonfüred, 28. April – 1. May, 2000 (80 participants)

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