ANNUAL REPORT

1997



RESEARCH INSTITUTE FOR SOLID STATE PHYSICS 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 1997 Edited by L. Csillag, J. Kollár, G. Konczos, B. Selmeci Closed on 1st December, 1997

Dear Reader,

It is my pleasure to hand over the 4th Volume of the yearbook of the Research Institute for Solid State Physics. This booklet summarises our activities for the year 1997.

Our institute has been founded by the Hungarian Academy of Sciences in 1981 as part of the Central Research Institute for Physics. Since 1992 we are an independent institute involved to a larger extent in basic and to a smaller one in applied research.

Our basic research is in theoretical and experimental solid state physics, in materials sciences, in the interaction of light with matter and in certain fields of laser physics while the applied work is carried out in optical thin films, laser applications, non-destructive testing and special material technologies. Some of our research is connected with unique large or medium sized facilities like our research reactor where neutron scattering experiments are performed.

The financial conditions have not been too rosy also this year, since the budgetary constraints are still strong in the country. The "seven thin years" have not yet come to an end. Fortunately, however, the grants obtained from the National Research Found covered the minimal needs of research. Significant support has been won from the National Committee for Technological Development for instrumentation.

International cooperation plays a vital role in our work. We have living contacts with a great number of research institutions and universities, being partners in common research, opening access to special research facilities and to valuable information. In about 70% of our publications there are foreign co-authors showing the significant role of these contacts. The different EU, NATO and other international grants play also a non - negligible role in the support of our research. It is expected that the share of these resources in our budget will increase with the evolution of the integration process in our country.

Our institute has traditionally been participating in gradual and even more strongly in postgradual education. Details of this activity are also given in this booklet.

An important measure of our results is the number of scientific publications and their quality (impact). I am glad to report that our publication activity has been on the level of the previous years in spite of all our difficulties. The 150 published papers in international journals or conference proceedings are similar to the numbers in previous years.

May I hope that this booklet gives useful information to the reader. Our scientists are ready to supply further information, if needed. This may be helped by the e-mail addresses given at the end of each chapter. Our WWW home page may serve the same purposes.

Budapest 1st December 1997.

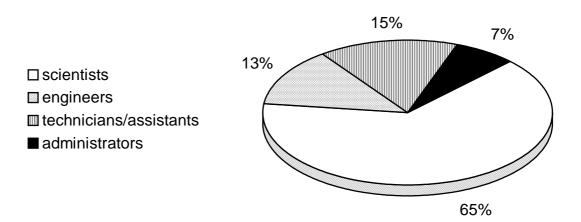
Norbert Kins

Norbert Kroó Director

Key figures

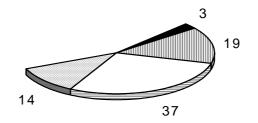
Permanent staff of the Institute: 130 employees. Its distribution:

a) by professions:



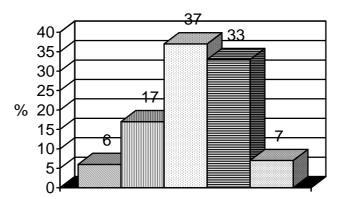
b) by scientific titles/degrees:





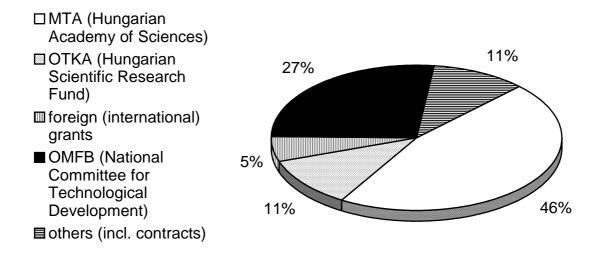
c) by ages:

under 30 years
 30-40 years
 40-50 years
 50-60 years
 over 60 years

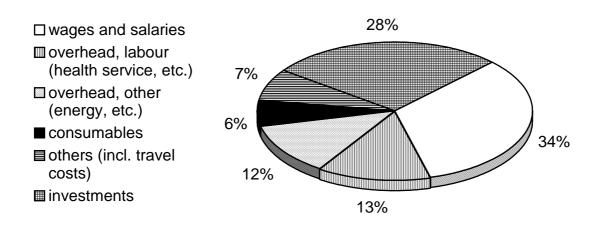


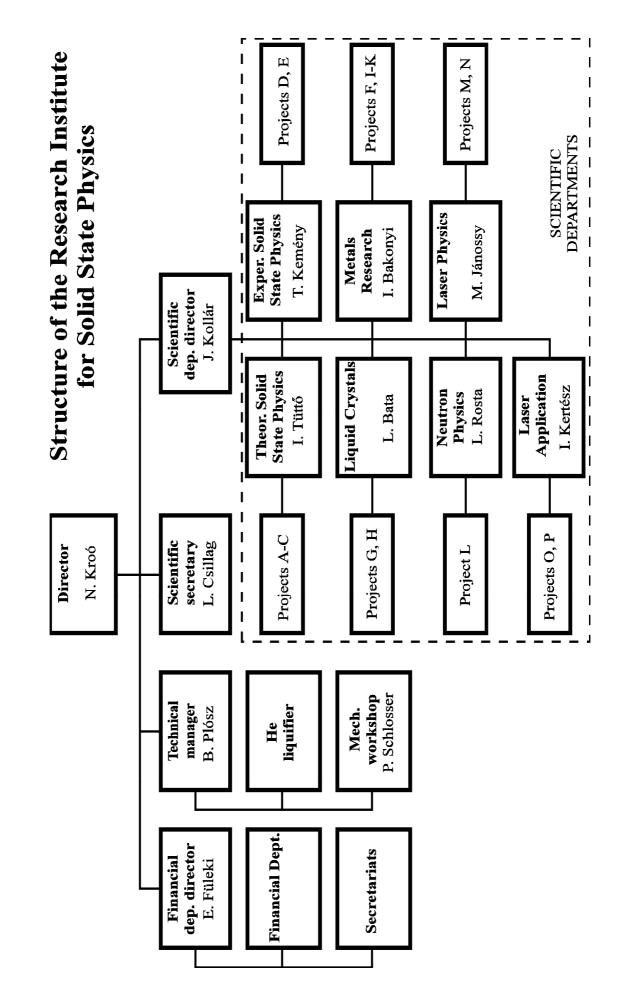
Financial management

a) Sources of operation costs:



b) Distribution of expenditures:





A. STRONGLY CORRELATED SYSTEMS

<u>J. Sólyom</u>, G. Fáth, Ö. Legeza, K. Penc, K. Vladár, F Woynarovich, A. Zawadowski⁺

Low dimensional magnetic models. — We continued our study of the physical properties of the so-called magnetic ladder systems. We have considered anisotropic two-leg ladder models with S=1/2 and S=1 spins on the rungs, using the density matrix renormalization group (DMRG) method. We have generalized the numerical procedure to allow to take into account the symmetries of the models in order to reduce the dimension of the matrix to be diagonalized or to achieve better accuracy. We have determined the boundaries of the extended region in the parameter space, where the gapped Haldane phase exists. In our study of the scaling limit of the one dimensional XXZ Heisenberg chain we have found, that the limiting model possesses spin 1/2 massive particles, and possibly can be identified with the Sine-Gordon chain.

One-dimensional fermionic models. — We continued the study of the models defined through the relativistic limit of the Hubbard chain by investigating the scaling limit of the one dimensional attractive Hubbard model at less than half filling. Like in the half filled band case, also this model possesses both massive and massless dressed particles. Now, unlike the half filled case, only the massive particles are described by Bethe Ansatz type equations, nevertheless the massless excitations still fit into the framework of a conform field theory.

Theory of dissipative motion of heavy particles. — We studied the low temperature behaviour of two level systems (TLS) interacting with the conduction electrons in various models and approximations. We continued the study of the region below the Kondo temperature by the use of the model with electron spin degeneracy $N_f > 2$. The only stable fixed point and the exponents of the leading irrelevant operators are equivalent to those of the spin 1/2 Kondo model, but there are essentially more irrelevant operators in our case. We studied the role of the electron-hole symmetry in the low temperature behaviour of TLS, moreover the differences between the scaling methods starting from path integrals and Matsubara technique. We showed that the breaking of the electron-hole symmetry results in electron assisted tunneling, but the contribution cannot bring the system to the two-channel Kondo fixed point.

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Grants

OTKA¹ T 014443 Completely integrable 1-d systems (F. Woynarovich, 1994-1997)

⁺ Permanent position: Technical University of Budapest

¹ OTKA = Hungarian Scientific Research Fund

OTKA T 015870.	Models of strongly correlated low-dimensional electron systems
	(J. Sólyom, 1995-1998)
OTKA T 017128.	Theoretical study of dissipative motion of heavy particles
	(K.Vladár, 1995-1998)

Publications⁺

- A.1. Ö. Legeza, G. Fáth and J. Sólyom: Phase diagram of magnetic ladders constructed from a composite-spin model. *Phys. Rev.* **B55**, 291-298 (1997).
- A.2. P. Santini^{*}, G. Fáth, Z. Domanski^{*} and P. Erdős^{*}, Quantum fluctuations and anisotropy in quasi-one-dimensional antiferromagnets. *Phys. Rev.* B56, 5373-5379 (1997).
- A.3. F. Woynarovich and P. Forgács*: Scaling limit of the one-dimensional attractive Hubbard model: The half-filled band case. *Nuclear Physics* **B498** 565-603 (1997).
- A.4. G. Zaránd* and K. Vladár: Low temperature dynamics of an N_f -flavor two level system in a metal: Equivalence with the N_f -channel Kondo model in the $(1/N_f)^2$ order. *Phys. Rev. Letters* **76**, 2133-2136 (1996).
- A.5. A. Zawadowski, G. Zaránd*, P. Nozières*, K. Vladár and G. T. Zimányi*: Instability of the marginal commutative model of tunneling centers interacting with metallic environment. Role of the electron-hole symmetry breaking. *Phys. Rev.* B57, 12947-12960 (1997).
- A.6. W. Stephan^{*} and K. Penc: Dynamical density-density correlations in onedimensional Mott insulators. *Phys. Rev.* **B54**, R17269-17272 (1996).
- A.7. J. Favand^{*}, S. Haas^{*}, K. Penc, F. Mila^{*} and E. Dagotto^{*}: Spectral functions of one-dimensional models of correlated electrons. *Phys. Rev.* B55, R4859-4862 (1997).
- A.8. K. Penc, K. Hallberg^{*}, F. Mila^{*} and H. Shiba^{*}: Spectral functions of the 1D Hubbard model in the U→∞ limit: How to use the factorized wave function. *Phys. Rev.* B55, 15475-15488 (1997).
- A.9. F. Mila^{*} and K. Penc: Spectral-Function and Self-Energy of the One-Dimensional Hubbard-Model in the U→∞ Limit. Z. für Phys. B 103, 201-203 (1997)
- A.10 B. Normand^{*}, K. Penc, M. Albrecht^{*} and F. Mila^{*}: Phase diagram of the S=1/2 frustrated coupled ladder system. *Phys. Rev.* **B56**, R5736-5739 (1997).

⁺The *Annual Report* contains publications appeared or accepted by the publishers in the period 1 December 1996 - 30 November 1997

^{*} The author is not a member of the Research Institute for Solid State Physics staff

- A.11 K. Penc and M. Serhan^{*}: Finite-temperature spectral functions of strongly correlated one-dimensional electron systems. *Phys. Rev.* B56, 6555-6558 (1997).
- A.12. Ö. Legeza and J. Sólyom: Stability of the Haldane phase in anisotropic magnetic ladders. *Phys. Rev.* **B**, accepted for publication
- A.13. G. Zaránd* and K. Vladár: Orbital Kondo effect from tunneling impurities. *Int. J. Mod. Physics*, accepted for publication.

Conference proceeding

 A.14. F. Mila* and K. Penc: Correlation Effects in Quasi-One Dimensional Organic Conductors: A Microscopic Point of View. In: *Proc. Conf. "Correlated Fermions and Transport in Mesoscopic Systems"*, ed. T. Martin, G. Montambaux and J. Tran Thanh Van (Frontieres, 1996), p. 105.

B. COMPLEX SYSTEMS

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

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

Phase transitions. — We have studied the effect of quenched randomness on the nature of phase transitions, both for classical and quantum systems. The surface critical behaviour of the classical random bond ferromagnetic Ising model has been studied with the result that the surface magnetization exponent is robust against dilatation while exponents of correlation length and decay of critical surface are subject of strong, logarithmic corrections. The random transverse-field Ising spin chain, trated by analytical and numerical methods, has offered the possibility of studying density profiles in a geometrically constrained disordered system at a quantum phase transition. The critical magnetization- and energy density profiles were found to follow predictions of conformal invariance, although the system is not conformally invariant. A scaling theory for dynamical correlations has also been developed and justified numerically.

At the so called parity conserving phase transition point of non-equilibrium kinetic Ising models in one dimension two non-equilibrium critical dynamical exponents (the persistency-exponent and the exponent of the two-time autocorrelation function) have been determined numerically for the total magnetisation. The results show that the PC transition has strong effect : the Glauber-Ising process becomes non-Markovian.

Chaos. — We have investigated the problem of chaotic diffusion and have shown that the diffusion constants exhibit anomalous behaviour in the critical state.

Quantum systems. — A work has been presented on the tunnelling of the magnetisation in the presence of an alternating magnetic field, showing that this latter can only hamper the magnetisation.

Theory of Bose-condensed gases. — Bose-condensed gases have come into the focus of interest lately. In describing their behaviour we have determined the spectrum of the elementary excitations in the whole energy region. Moreover, the theory of inelastic scattering of light on the system has been developed and an investigation of nonlinear chaotic effects in the classical limit has been carried out.

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Grants:

OTKA T023642 Phase transitions in quasi-crystals, aperiodic and disordered systems (F. Iglói, 1997-2000) OTKA T17493 Theory of random processes and complex structures (P

OTKA T17493 Theory of random processes and complex structures (P. Szépfalusy, 1995-1998)

⁺ Permanent position: Eötvös Loránd University, Budapest

OTKA T14855 Phase transitions and spectral problem in quantum systems (A. Sütő, 1995-1998)

OTKA T023791 Nonequilibrium phase transitions (N. Menyhárd, 1997-2000)

Publications

- B.1. F. Iglói and H. Rieger^{*}: Density Profiles in Random Quantum Spin Chains. *Phys. Rev. Lett.* **78**, 2473-76 (1997)
- B.2. L. Turban^{*} and F. Iglói: Off-diagonal Density Profiles and Conformal Invariance. J. Phys. A30, L105-L111 (1997)
- B.3. F. Iglói and G. Palágyi^{*}: Non-Universal Critical Behaviour in the Mean-Field Theory of Inhomogeneous Systems. *Physica* A240, 685-693 (1997)
- B.4. F. Iglói, L. Turban^{*}, D. Karevski^{*} and F. Szalma^{*}: Exact Renormalization Group Study of Aperiodic Ising Quantum Chains and Directed Walks. *Phys. Rev.* B56, 11031-11052 (1997)
- B.5. H. Rieger^{*} and F. Iglói: Quantum Critical Dynamics of the Random Transverse-Field Ising Spin Chain. *Europhys. Lett.* **39**, 135-140 (1997)
- B.6. L. Gránásy and F. Iglói: Comparison of Experiments and Modern Theories of Crystal Nucleation. J. Chem. Phys. 107, 3634-3644 (1997) (see also E.2.)
- B.7. W. Selke^{*}, F. Szalma^{*}, P. Lajkó^{*} and F. Iglói: Surface Critical Behavior of twodimensional Dilute Ising Models. *J. Stat. Phys.* **89**, 1079-1089 (1997)
- B.8. J. L. van Hemmen^{*} and A. Sütõ: ac-hampered tunnelling of the magnetisation, *J. Phys.* A: Cond. Mat. **9**, 3089-3097 (1997)
- B.9. Z. Kaufmann^{*}, H. Lustfeld^{*}, A. Németh^{*} and P. Szépfalusy: Diffusion in Normal and Critical Transient Chaos. *Phys. Rev. Letters* **78**, 4031-4034 (1997).
- B.10. N. Menyhárd and G. Ódor^{*}: Non-Markovian Persistence at the Parity-Conserving Point of a One-Dimensional Non-Equilibrium Kinetic Ising model. *J. Phys.* A, accepted for publication
- B.11. A. Csordás, R. Graham^{*} and P. Szépfalusy: Semiclassical wave functions and energy levels of Bose-condensed gases in spherically symmetric traps. *Phys. Rev.* A, accepted for publication
- B.12. M. Fliesser^{*}, A. Csordás, P. Szépfalusy and R. Graham^{*}: Hydrodynamic excitations of Bose Condensates in anisotropic traps. *Phys. Rev.* A, accepted for publication
- B.13. M. Fliesser^{*}, A. Csordás, R. Graham^{*} and P. Szépfalusy: Classical quasiparticle dynamics in trapped Bose condensates. *Phys. Rev.* A, accepted for publication

C. ELECTRONIC STATES IN SOLIDS

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

We have finished our studies on the equilibrium bulk properties of **light actinides**. It has been shown that the unexpectedly large atomic volume for α -Pu can be ascribed to the presence of low coordinated sites in the structure where the f-electrons are close to the onset of localization and the charge density is very low in the interstitial region. In this case the *local density approximation* is not able to describe properly the exchange-correlation effects, while the accuracy of the *generalized gradient approximation* is satisfactory for this system as well.

Our recently developed **full charge density scheme** has been applied to study the **surface electronic states** of metals. In the new version of the method the kinetic energy is also corrected due to the presence of non-spherically symmetric charge density components. We have established a database of surface energies for low index surfaces of 60 metals in the periodic table. The data may be used as a consistent starting point for models of surface science phenomena. The calculated surface energy anisotropies are compared with other density functional theory results and applied in a determination of the equilibrium shape of nano-crystals of Fe, Cu, Mo, Ta, Pt and Pb. Furthermore, using the self-consistent jellium model of metal surfaces we investigated the accuracy of a number of semi-local kinetic-energy functionals. Based on this study, we propose a simple one parameter Padé's approximation which reproduces the exact Kohn-Sham surface kinetic energy over the entire range of metallic densities.

We studied the magnetic properties of surfaces and interfaces, by performing fullyrelativistic spin-polarized local spin density calculations based on the Screened KKR method. The study of the ground state and the magnetic anisotropy of antiferromagnetic fcc Fe/Cu(001) over-- and interlayers revealed, that contrary to a previous study of the ferromagnetic state, for all considered cases, namely up to seven layers of Fe, the magnetization is oriented along the surface normal. The crucial role of the volume (lattice spacing) on the formation of the antiferromagnetic ground state is also studied. This calculation presented an excellent opportunity to compare the magnetic anisotropy energies in ferromagnetic Fe the main contribution comes almost exclusively from the the layers closest to the substrate and to the surface, in antiferromagnetic state this effect is much less pronounced, all layers contribute almost equally to the Magnetic Anisotropy Energy.

We also suggested a new mechanism for explaining the tilt of the magnetization away from the surface normal in certain magnetic ultra--thin films. Our arguments are based on a simple classical spin Hamiltonian in which the magneto-crystalline surface anisotropy is described by $H_a = -\sum_i \lambda_i (s_i^z)^2 + \sum_i \gamma_i (s_i^z)^4$, where λ_i and γ_i are nonnegative phenomenological constants, s_i^z denotes the z-component (normal to the surface) of the spin at the site labelled by i. By studying the ground state of this model, in contrast to the usual explanation which attributes the experimentally observed tilted magnetization to the fourth order term involving γ_i , we show that the second order term alone can lead to this interesting phenomenon. Our explanation implies that the magnetization of the successive layers are not collinear. We showed that

⁺ Permanent position: Technical University Budapest

experimentally observed orientational transition of the Co/Au(111) system can be recovered by our model.

We have investigated the consequences of the dispersion of the energy bands in the **charge- and spin-density wave states** of highly anisotropic metals. Such dispersion becomes important with increasing deviations from perfect nesting, and leads to differences between the gaps as sampled by transport and optical measurements. We discussed the available experimental results obtained in a variety of materials with different band-structure anisotropy, and found excellent agreement with our simple theory.

As a continuation of our previous research on band ferromagnetism we studied the conditions for the appearance of an itinerant **ferromagnetic phase in lattice fermion models**. Several basic scenarios were identified:

- 1. single-orbital Hubbard models may become ferromagnetic in close-packed lattices if the hopping amplitudes satisfy a certain sign rule;
- 2. the double exchange mechanism in degenerate Hubbard models works for any lattice structure, and
- 3. ferromagnetism between quarter and half-filling in Anderson and Kondo lattice models, in which case ferromagnetism competes with the collective Kondo state. It is possible that these scenarios are interrelated in a more general framework which is under current study.

We studied the consequence of a nonconventional barrier at a **superconductorsuperconductor interface**. Due to the forward scattering part of the barrier, a strong nonlinearity shows up in the Andreev scattering. We have shown that this nonlinearity may be responsible to the anomalous behaviour of the Josephson effect in the unconventional superconductors.

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Levente Vitos	lv@power.szfki.kfki.hu

Grants

OTKA T14201	Theory of phase diagrams of heavy fermion systems (P. Fazekas, 1994-1997)
OTKA T16740	Electronic states in complex structures (solids, surfaces and interfaces) (J. Kollár, 1995-1998)
OTKA T020030	Interacting electrons in low dimensions (A. Virosztek, 1996- 1999)
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 T019045 Collective excitations in unconventional superconductors (I. Tüttő, 1996-1999)

Publications

- C.1. L. Vitos, J. Kollár and H.L. Skriver^{*}: Ab initio full charge density study of the atomic volume of α-phase Fr, Ra, Ac, Th, Pa, U, Np and Pu. *Phys Rev.* B55, 4947-4952, (1997)
- C.2. L. Vitos, J. Kollár and H.L. Skriver^{*}: Full charge density scheme with a kinetic energy correction: Application to ground-state properties of the 4d metals. *Phys Rev.* **B55**, 13521-13527, (1997)
- C.3. J. Kollár, L. Vitos and H.L. Skriver^{*}: Anomalous atomic volume of α-Pu. *Phys Rev.* **B55**, 15353-15355, (1997)
- C.4. L. Szunyogh^{*}, B. Újfalussy, and P. Weinberger^{*}: Magnetic structure and a nisotropy in Fe/Cu(001) over- and interlayers considering antiferromagnetic interlayer coupling. *Phys. Rev.* B **55**, 14392--14396 (1997)
- C.5. G. Mihály, A. Virosztek and G. Grüner^{*}: Thermal and optical gaps in nearly one-dimensional compounds. *Phys. Rev.* B **55**, R13456-13459 (1997)
- C.6. P. Fazekas: Band ferromagnetism versus collective Kondo state in lattice fermion models. *Phil. Mag.* B **76**, 797-806 (1997).
- C.7. P. Fazekas and K. Itai: Collective Kondo effect in the Anderson-Hubbard lattice. *Physica* B **230-232**, 428-430 (1997).
- C.8. S. Daul^{*}, P. Pieri^{*}, M.Dzierzawa^{*}, D. Baeriswyl^{*}, and P. Fazekas: Low density ferromagnetism in a one-dimensional Hubbard model. *Physica* B **230-232**, 1021-1023 (1997).
- C.9. L. Vitos, J. Kollár and H.L. Skriver^{*}: LDA versus GGA: full charge density study of the atomic volume of the light actinides. *J. Alloys and Compounds,* accepted for publication
- C.10. L. Vitos, A.V. Ruban^{*}, H.L. Skriver^{*} and J. Kollár: The surface energy of metals. *Surface Science*, accepted for publication
- C.11. L. Vitos, H.L. Skriver^{*} and J. Kollár: Kinetic energy functionals studied by surface calculations. *Phys. Rev.* B, accepted for publication
- C.12. L. Szunyogh^{*}, B. Újfalussy, C. Blaas^{*}, U. Pustogowa^{*}, C. Sommers, and P. Weinberger: Oscillatory behavior of the magnetic anisotropy energy in Cu(100)/Co_n multilayer systems. *Phys. Rev.* B, accepted for publication
- C.13. L. Udvardi^{*}, R. Király^{*}, L. Szunyogh^{*}, L. Denat^{*}, M.B. Taylor^{*}, B.L. Győrffy^{*},
 B. Újfalussy and C. Uiberacker^{*}: On Tilted Magnetization In Thin Films. *J. Magn. Magn. Mater.*, accepted for publication

C.14. P. Weinberger^{*}, C. Sommers^{*}, U. Pustogowa^{*}, L. Szunyogh^{*}, and B. Újfalussy: Ab-initio determination of magnetic interface coupling constants for magnetic multilayers. *J. Physique*, accepted for publication

Conference proceedings

- C.15. B. Újfalussy, L. Szunyogh^{*}, and P. Weinberger^{*}: Alloying aspects of the magnetic ground state and anisotropy of Fe/Cu thin film overlayers In: *"Properties of Complex Inorganic Solids"*. Edited by Antonios Gonis, Annemarie Meike and Patrice E. A. Turchi. Plenum Press, New York and London (1996), pp. 181-187
- C.16. B. Újfalussy, L. Szunyogh^{*}, and P. Weinberger^{*}: Magnetic anisotropy of Fe/Cu(100) over- and interlayers, In: *Proc. of the MRS Spring Meeting, Symposium Magnetic Multilayers, San Francisco, CA, USA, March 31 - April* 4 (1997), accepted for publication

Book chapters

C.17. L. Vitos, J. Kollár and H.L. Skriver^{*}: Bulk properties of the light actinides from first principles. In *Actinides and the Environment*, NATO ASI Series, Eds. P.A. Sterne, A. Gonis, A.A. Borovoi, Kluwer Academic Press, (1997), pp. 212-216

D. NON-EQUILIBRIUM ALLOYS

<u>I. Vincze</u>, J. Balogh, L. Bujdosó, D. Kaptás, T. Kemény, L.F. Kiss, Gy. Mészáros, B. Sas, E. Sváb

Granular systems and spin glasses. — Magnetic systems with a considerable amount of irregular interfaces were investigated by ⁵⁷Fe Mössbauer spectroscopy. Chemically homogeneous ferromagnets around the percolation threshold composition of disappearing magnetism and chemically heterogeneous alloys prepared by nanocrystallization of amorphous alloys belong to this class of materials. Low temperature and high field measurements were performed on nanocrystalline FeZrBCu alloys, on ball-milled Fe with nano-size grains and on melt-quenched amorphous Fe-Zr and Fe-Y alloys in order to clarify the origin of the large high-field susceptibility and to investigate the common features of the approach to magnetic saturation.

In the melt spun amorphous Fe-Y alloys with 15-60 at% Y content the reduced values of the bulk magnetic high-field susceptibility and the equivalent quantity determined from the Fe hyperfine field measured by Mössbauer spectroscopy were found to be similar which rules out the hypothesis of a frustrated magnetic structure as the explanation of their spin glass and re-entrant spin glass-like magnetic behaviour.

In the magnetically inhomogeneous nanocrystalline FeZrBCu alloys the Curie point of the residual amorphous phase was determined by Mössbauer spectroscopy measurements and no significant enhancement of T_c due to the supposed polarization effects of the ferromagnetic nanocrystalline body centered cubic (*bcc*) phase was found in these few nanometer size amorphous parts. The nanocrystalline *bcc* phase is a non-equilibrium Fe solid solution with Zr and B. The approximately two atomic layer thick interfacial region of these nanocrystalline phases was investigated and found to be responsible for the magnetic coupling of the ferromagnetic grains. The composition of the residual amorphous matrix was found to be Fe₂(B, Zr) and its preparation and investigation in bulk form has been started. Besides the academic interest, the study of the nanocrystalline materials is also aimed to develop new compositions with enhanced soft magnetic properties (high initial permeability and low power loss) applicable in sensors and transformers.

Magnetic viscosity. — Magnetic viscosity was measured for amorphous Fe_{100-x}Zr_x ($7 \le x \le 12$) alloys in the spin-glass state as a function of magnetic field (0 < H < 500 Oe) and temperature (4.2 < T < 60 K). The viscosity field, H_v , deduced from these measurements is independent of H and decreases with increasing temperature as $(1/T)^{2.0\pm0.3}$ for all the alloys. The activation volume, V_a , calculated from H_v varies with the temperature as $T^{3.0\pm0.3}$. The reduced coercivity, $h_c = H_c/2\pi M_s$ (H_c being the coercivity and M_s the saturation magnetization) as a function of D_a , the characteristic size calculated from the activation volume, falls approximately to a common curve for all the alloys. This dependence decreases with increasing D_a as $(1/D_a)^{2.0\pm0.2}$. Such a size dependence of the coercivity hints at a curling-type nucleation mechanism of domains in the spin-glass state of the amorphous Fe-rich Fe-Zr alloys.

Relaxation. — The reversible structural relaxation of $Fe_{37.5}Ni_{37.5}B_{25-x}P_x$ (x = 0, 3, 6, 16, 25) and $Fe_{37.5}Ni_{37.5}B_{25-y}Si_y$ (y = 0, 5, 10, 15) metallic glasses was investigated by differential scanning calorimetry and resistivity measurements, using the activation energy spectra model . From the deduced activation enthalpy spectra for these amorphous alloys, it is concluded that possibilities for atomic movements with characteristic activation energies are created by the substitution of B with P or Si. It is shown that at least one Gaussian contribution to the activation energy spectrum appears on increasing P or Si content, superimposed on an exponential part previously found for Fe-Ni-B glasses. The amplitude of the Gaussian function increases with increasing P or Si content. According to isothermal resistivity measurements, for P substitution the reversible atomic rearrangements connected to the Gaussian contribution increase the resistivity while those associated with the exponential part decrease it. For Si substitution both processes decrease the resistivity.

Ball milling and solid state reaction studies. — Solid state amorphization was studied in the Fe-B system. Diffusion amorphization was shown to exist in the 32-47 at% B concentration range by examining nanostructured multilayers. On the other hand FeB and Fe₂B cannot be amorphized by mechanical grinding. When the stoichiometry is changed, either by contamination during mechanical milling or by the mechanical alloying of Fe + FeB or Fe + Fe₂B powder mixture, an amorphous alloy is formed with composition close to Fe₈₀B₂₀. The results show that compositional changes are more effective in the amorphization than heavy deformation or diffusion. The studies were extended to the mechanical crystallization of metallic glasses in the Fe-B system. By comparing the different behaviours observed in WC and steel containers, it was verified, that besides the usually assumed mechanical effects the steel tools introduce Fe-rich nuclei and this way dominantly influence the observed crystallization. The ball milling of amorphous ribbons used to form nanocrystalline materials was also investigated. It was established that the comminuted powder is a promising material for some soft magnetic applications.

Neutron scattering. — The metaloxides having the general formula AB_2O_4 (spinels) possess suitable combined electric and magnetic properties and therefore became very important for pure scientific and for many technological applications, as well. Investigating the structural consequences of ion implantation in insulators we became interested in spinel structures. Neutron diffraction measurement was performed on the FeAl₂O₄ spinel in a wide scattering angle range. Rietveld refinement was used to determine the cation distribution and the oxigen position parameter. It was established that the structure is a partly inverse spinel with a degree of inversion 18 %. The best fit resulted for the oxigen position parameter with 0.2632.

Neutron diffraction measurements were performed on rapidly quenched aqueous solution of ferrous-perchlorate of different concentrations. D_2O was used as solvent and the crystal water of Fe(ClO₄)₂.6H₂O was partly substituted by heavy water, in order to avoid the high incoherent scattering of hydrogen. After fast-freezing, the formation of hexagonal ice and an amorphous phase was observed for concentrations of 1.6 and 3.2 mol%, while for the 6.5 mol% concentration, the formation of a pure amorphous phase was obtained. Phase transitions were observed and analysed after heating the frozen samples in the temperature range of $-160^{\circ}C$ and $-25^{\circ}C$ with various heating rates. Starting from the amorphous state, formation of a viscous phase, thereafter at higher temperatures the formation of hexagonal ice and crystalline

structures were observed. Different crystalline structures were obtained by heating the fast-frozen samples at high or low heating rates.

Dynamic neutron radiography was used to test various new constructions of absorption-, and compression-type refrigerators with the aim of development. Radiography was applied for plant research by visualizing the water uptake and distribution during the germination of bean seeds. The quantitative analysis of the images showed three distinct zones: the absorption, evaporation and accumulation zones. The accumulation zone forming in the facing surfaces of the cotyledons may contribute to their opening. The time scale of the imbibitions, germination and primary root growth was identified.

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Grants

Copernicus COP 753 Manufacture, structure and properties of amorphous and
nanocrystalline materials (T. Kemény, 1995-1997)
OTKA I/7 T017456 The spin glass behaviour and its relation to the magnetic
properties of nanostructures. (I. Vincze, 1995-1997)
OTKA T020624 Photon- and electron-spectroscopic study of the interfaces of
layer structures (J. Balogh, 1996-1999)
OTKA T020962 Formation and magnetic properties of granular structures (T.
Kemény, 1996-1998)
OTKA I/7 T017129 Metastable systems investigated by neutron scattering (E. Sváb,
1996-1999)
OTKA T022413 Atomic and magnetic structure of nanosystems and interfaces
(I. Vincze, 1997-1999)
OTKA F020092 The investigation of near-surface layers by spectroscopic and
diffraction methods (D. Kaptás, 1996-1999)
AKP ² 96-137/6 Mössbauer spectroscopy of nanostructures and strongly
correlated electron systems (I. Vincze, 1996-1997)

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Articles

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- D.14. A. Böhönyey^{*}, G. Huhn^{*}, L.F. Kiss, A. Lovas , I. Gerõcs^{*}: Effect of metalloid substitution on the reversible structural relaxation of Fe-Ni-B(-P, Si) metallic glasses. *J. Non-Cryst. Solids*, accepted for publication

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

- D.27. M. Balaskó^{*}, E. Sváb: Kombinált roncsolásmentes anyagvizsgálati módszerek alkalmazása a KFKI kutatóreaktornál (Application of combined material testing methods at the KFKI research reactor, in Hungarian). *Anyagvizsgálók Lapja* **1-2**, 34-36 (1997)
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E. X-RAY DIFFRACTION

<u>G. Faigel,</u> G. Bortel, L. Gránásy, K. Kamarás, G. Oszlányi, S. Pekker, T. Pusztai, M. Tegze

Alkali fullerides. — The fullerenes are closed shell molecules containing only carbon atoms. The most abundant among them is the C_{60} molecule. Fullerenes can form a large variety of compounds with elements or other molecules. In the group of A_xC_{60} compounds (A=K,Rb,Cs x=1,3,4,6) there are materials with very interesting properties. Among them many superconducting materials (A_3C_{60}) with remarkably high critical temperature were found. In the last few years the polymeric forms of alkali C_{60} salts became the center of interest. The suggestion of the solid state ionic (2+2)cycloaddition polymerization of singly charged fulleride ions in AC₆₀ (A=K, Rb, Cs) salts established a new class of fullerene derivatives. This initiated an extensive study of their structure, of the mechanism of their formation, and of the thermodynamic and the most important physical and chemical properties of these phases. After finding the answers to most of the above questions, we could go further and produce polymers with different bonding configurations and with different dimensionality. For this reason we did quantum chemical calculations and analyzed the stability of various 1D and 2D polyanions with 1,2 and 4 sp³ carbons connected by either (2+2) cycloadduct or by single bonds. We found several stable phases such as Na₂RbC₆₀ and Na₄C₆₀. We also extended our experimental work into this direction. We synthesized the Na_4C_{60} which turned out to be a 2D polymer. Its structure and bonding configuration was determined from x-ray powder diffraction using Rietveld analysis.

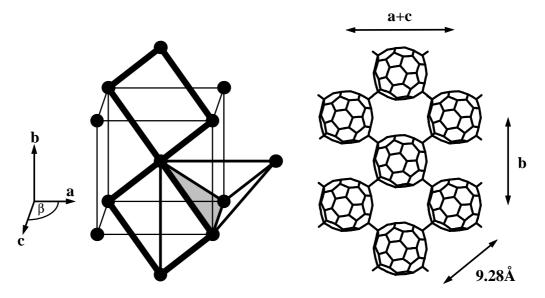


Fig.1. Molecular arrangement of Na₄C₆₀

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. In the last decade the introduction of soft x-ray instead of visible light tremendously improved the resolution which reached a few hundred angström. An other line in holography, based on the inside source concept, was suggested recently.

We have applied this concept for the case of fluorescent x-rays emitted by a single crystal. We were the first to demonstrate experimentally the feasibility of x-ray holography with atomic resolution on SrTiO₃. Shortly after our work an other, closely related method the "inverse" holography (using the inside detector concept) was put forward. We integrated this into our research project. We developed an experimental setup which is capable of taking normal and "inverse" holograms of the same sample without realigning the optics or repositioning the sample. Using this setup more holograms on different materials such as NiO and Ge were taken. We also worked on the closely related Kossel lines and standing waves. We have shown that it is possible to detect these patterns using external x-ray excitation. Further it was demonstrated that structural parameters can be obtained from these patterns.

Nucleation theory. — We investigated the applicability of five non-classical nucleation theories. Experimental nucleation rates on six substances, including hydrocarbons, a molten metal and oxide glasses, were analyzed in terms of phenomenological and density functional approaches. It is demonstrated that of the nucleation models we considered, only the semiempirical density functional approach and the phenomenological diffuse interface theory proposed by us are fully consistent with the data. The other models (the self-consistent classical theory and the detailed molecular theories) did not provide a satisfactory fit with experiment. The failure/success of these approaches were discussed in terms of the applied approximations. We developed a numerical model of first-order phase transformations that considers the mutual blocking of growing particles up to all relevant orders. It is applicable for the growth of fixed number of particles, or to simultaneous nucleation and growth processes, in any space dimensions, even in the case of highly anisotropic growth. Monte Carlo simulations were carried out in two dimensions for steady state nucleation and random elliptical growth. It is demonstrated that the Johnson-Mehl-Avrami-Kolmogorov model is not applicable under such circumstances.

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Grants

OTKA T016057	Preparation and structural, optical and thermal studies of fullerenes
	and related materials (G. Faigel, 1995-1998)
OTKA T017485	Theoretical investigation of nucleation processes (L. Gránásy,
	1995-1997)
OTKA T019139	The study of polymer fullerides and other crystalline C_{60}
	compounds (S. Pekker, 1996-1999)
OTKA T022041	X-ray holography (M. Tegze, 1997-2000)
OTKA F020027	X-ray studies of anisotropic and modulated structures (G. Oszlányi,
	1997-2000)

- AKP 96 225 /12 Atomic resolution holography using nuclear gamma decay (G. Faigel, 1996-1997)
- AKP 96/2 450 2,2 Structural study of new type of equilibrium and non-equilibrium molecular systems (M. Tegze, 1997-1998)
- U.S.-Hungarian Joint Fund 225 Single crystal C₆₀ spectroscopy (S. Pekker, 1994-1997)
- U.S.-Hungarian Joint Fund 271 Optical properties of high-T_c crystals (K. Kamarás, 1994-1997)
- U.S.-Hungarian Joint Fund 431 Structural study of C_{60} compounds (G. Faigel, 1995-1997)

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F. CHARGE- AND SPIN-DENSITY WAVES

G. Kriza and G. Mihály⁺

Symmetry-breaking ground states in quasi-one-dimensional metals. — It has been demonstrated that with increasing anisotropy, the affinity of metals towards the formation of a symmetry-breaking ground state is also increasing. A special class of these ground states is encountered in quasi-one-dimensional conductors when both the electron-electron and electron-phonon interactions are important in determining the ground state properties. The textbook example is the so-called spin-Peierls (SP) state when the electrons of a half-filled band form singlet pairs accompanied by a perioddoubling lattice distortion. There is a renewed interest in these systems because of the discovery of SP ground state in CuGeO3 on the one hand, and some important theoretical developments on the other hand. We have tested these new ideas by NMR measurements over a broad range of magnetic fields in the SP state of the organic conductor (TMTTF)₂PF₆. We have shown that similarly to CuGeO₃, in high magnetic field, the SP system lowers its energy by the formation of an array of spin-carrying topological defects. We have pointed out, however, that the structure of these topological defects is different from those observed in $CuGeO_3$, and cannot be described by the Shu-Scrieffer-Heeger treatment adapted to the latter system.

Spin-density-wave fluctuations in Bechgaard-salts. We have continued the NMR investigation of collective spin-density wave (SDW) excitations in the quasi-one-dimensional Bechgaard salts by investigating the effect of controlled disorder on the spin-lattice relaxation. The experiments have been performed on the system $(TMTSF)_2(AsF_6)_{1-x}(SbF_6)_x$. We have shown that both the NMR relaxation properties and dielectric properties can be interpreted taking into account the interaction of the collective phase mode with the point defects of the crystal lattice.

Phase diagram of magnetic-field-induced spin-density waves. — We have investigated the pressure–magnetic field phase diagram of magnetic-field-induced spin-density waves (FISDW) in (TMTSF)₂PF₆. We have shown that the behavior close to the critical pressure for FISDW formation cannot be interpreted in the usual quasi-two-dimensional picture and the interactions in the third spatial dimension also have to be taken into account.

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Grants

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OTKA–NWO (The Netherlands): Electronic correlations in alkali metal fullerides (A. Jánossy, 1995-1999)

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

Publications

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G. LIQUID CRYSTAL RESEARCH

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

Study of ferroelectric liquid crystals. — A new set-up was built to study the rheology and other physical properties of columnar liquid crystals.

Quantitative electro-optical studies were carried out on smectic phases of chiral materials consisting of achiral banana shaped molecules. First in the literature we could obtain uniform alignment of smectic phases of banana shaped molecules and found evidence of reversible electro-optical switching of a racemic antiferroelectric phase.

Silica particle aggregates in liquid crystal matrix were studied in collaboration with the Neutron Physics Department. We have performed small angle neutron scattering studies and found that a few percent of SiO₂ particles dispersed in smectic liquid crystals results in a memory effect in the alignment of the liquid crystal matrix. Details of the memory effects were measured in Saclay at the Laboratoire Léon Brillouin on the G-43 triple-axis spectrometer ("VALSE") equipped with a multi-detector system for small angle scattering mode. The studies indicate that the silica particles form loosely connected porous aggregates.

Synthesis of chiral liquid crystals and their labelling by stable isotope. — Some novel chiral monomeric liquid crystals have been prepared as precursors of new polymeric liquid crystals. In some cases deuterium labelling was introduced into the core of the monomers offering the possibility to study the molecular dynamics by ²H NMR spectroscopy and neutron diffraction in different mesophases. Furthermore some new banana shaped molecules were prepared too for studying the chemical structures and physical properties of liquid crystalline materials.

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Grants:

OTKA T016152 Liquid crystal research (L. Bata, 1995-1998)
OTKA T023102 Investigation of physical properties of columnar and cubic
mesophase (A. Jákli, 1997-2000)
Volkswagen Foundation (German-Hungarian bilateral) Study of ferroelectric
columnar phases (A. Jákli, 1997-1998)
ERBIC15CT960744 INCO Copernicus EC Research Network: Novel techniques
and models for the surface treatment of liquid crystals with optical
applications (A. Jákli, 1997-1999)
OTKA T022772 Viscoelastic properties of smectic liquid crystals (N. Éber, 1997-
2000)
OTKA T020905 Deuterium labelling of liquid crystals (K. Fodor-Csorba, 1996-
1999)

Publications

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- G.5. D.Z. Obadovic^{*}, L. Bata, T. Tóth-Katona, A. Bóta^{*}, K. Fodor-Csorba, A.Vajda and M. Stancic^{*}: Structural properties of the ferroelectric liquid crystal mixtures based on the homologous series of alkoxyphenyl alkoxy benzoates. *Mol.Cryst. Liq.Cryst.* **303**, 85-96 (1997). (see also H.5.)
- G.6. A. Vajda, K. Fodor-Csorba, L. Bata, T. Paksi^{*}, Zs. Kakas^{*}, I. Jánossy and J. Hajtó^{*}: Phase Diagrams and Electrooptical properties of novel ferroelectric mixtures. *Mol.Cryst.Liq.Cryst.* 289, 89-102 (1996) (see also H.3.)
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Others (technical digests, papers in Hungarian, etc.)

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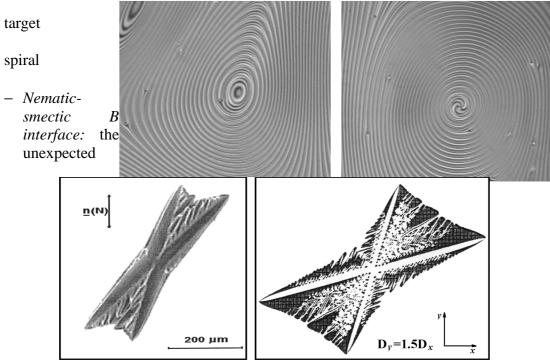
H. INSTABILITIES AND NONLINEAR PHENOMENA IN LIQUID CRYSTALS

<u>Á. Buka</u>, T. Börzsönyi, I. Jánossy, T. Tóth-Katona

Pattern formation.

- Oscillatory shear induced instabilities: the spatial and temporal director distribution (basic state) was measured optically and calculated from the nematohydrodynamic equations. At a critical amplitude a transition to a stationary roll pattern was observed and the threshold was compared with the result of the linear stability analysis of the basic state.

Phase waves (targets and spirals) emerging from a centre were generated after the homeotropically aligned nematic has undergone a bend Freedericksz-type distortion with an in-plane director component which is free to rotate.

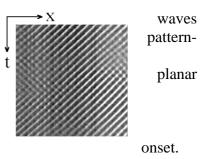


experimental phenomenon, that dendritic tips grow faster into the direction of lower heat diffusion (leading to shapes without reflection symmetry) was interpreted and reproduced by simulations.

experiment

simulation

 Viscous fingering: a new experimental setup was constructed to study Saffman-Taylor instability of a liquid crystal - air interface. Special care was taken of controlling the excess pressure precisely. Preliminary experiments have been carried out to study the influence of the viscosity on the morphology. The effective viscosity is regulated by an applied electric field. - Electrohydrodynamic instabilities: travelling (see the space-time diagram) as the primary forming instability were observed over the full conductive range of applied frequencies in the nematic Phase 5 (Merck). A theory - weak electrolyte model - was developed and a good agreement was found between the predicted and measured velocity of the travelling waves at



Non-linear optics.

- Laser-induced effects in liquid crystals: The investigation of laser-induced phenomena in dye-doped liquid crystals was continued. In particular, azo-dyes have been investigated that exhibit trans-cis isomerisation. A method was worked out to determine the absorption coefficients and dye order parameters of the two isomers separately. It was shown that the light induced trans-cis equilibrium depends on the polarization state of the beam. On the basis of this observation, the anomalous angular dependence of optical reorientation, observed earlier, was explained.

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Grants:

OTKA T-014957 Structure formation in non-equilibrium, complex systems (Á. Buka, 1995-1998)

- OTKA T-024098Laser induced phenomena in smectic liquid crystals (I. Jánossy, 1997-2000)
- OTKA F-022771 Interfacial patterns and convective instabilities (T. Tóth-Katona, 1997-2000)
- Volkswagen Foundation (German-Hungarian bilateral) Pattern formation in liquid crystals (Á. Buka, 1997-1998)

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Publications

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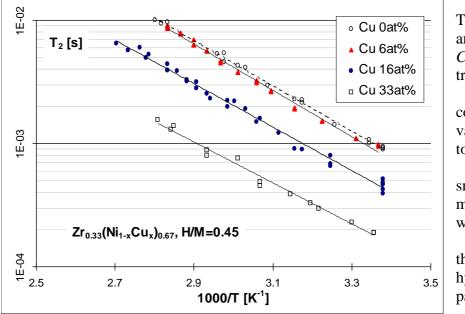
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I. METAL PHYSICS

<u>K. Tompa</u>, I. Bakonyi, M. Bokor⁺, Cs. Hargitai, Gy. Lasanda, T. Marek⁺, J. Tóth, E. Tóth-Kádár

Amorphous alloy - hydrogen systems. — In the study of metal-hydrogen ¹H spinspin relaxation time (T_2) and complementary hydrogen content, NMR spectrum width and spin-lattice relaxation time (T_1) have been measured in $\mathbf{Zr}_{\mathbf{y}}(\mathbf{Ni}_{1-x}\mathbf{Cu}_x)_{1-\mathbf{y}}$ -H ternary amorphous alloys of different hydrogen content at $0 \le x \le 33$ at % **Cu** and y = 33, 50 and 67 at % **Zr** concentrations using *Carr-Purcell-Meiboom-Gill*, solid-echo and saturation recovery pulse sequences, respectively. At high hydrogen contents the T_2 depends on both the **Zr** and **Cu** content, but that is independent of the hydrogen content. The differences in the spin-spin relaxation behaviours can be attributed to the substantial change of correlation time (represented by the intercept of the line in the Fig.) and not to the change of activation energy(represented by the slope of the line in the Fig) or local fields. The measurements were made in the "motional narrowing" state, consequently the quantities are averaged to the diffusion motion of protons taking part in this process.



The normalized amplitude of the **CPMG** echotrain gives the hydrogen content. the value has turned to be systematically smaller than that measured by weight increase, demonstrating that not all the hydrogen takes part in the diffusion

process.

Transition metal complexes. — Continuing the study of transition metal complexes ¹⁹F NMR spectra and spin-lattice relaxation times (T_1) were measured in $[Zn(ptz)_6](BF_4)_2$ (ptz = 1-*n*-propyl-1H-tetrazole) and in the spin-crossover complex $[Fe(ptz)_6](BF_4)_2$ between room temperature and 2.2 K on polycrystalline samples. The characteristics of the molecular motions of the BF₄ group (the correlation times and activation energies, respectively). were evaluated . For both complexes the same dynamics was found, which was expected because of the isomorphic structure of the two complexes. Similarly to the proton NMR results, clear signs of presence of high-

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spin state Fe^{2+} ions were detected. The result shows that there are Fe^{2+} ions remained in the high-spin state even at the lowest temperatures.

Metastable metallic phases. — As a continuation of our studies on Fe-, Co- and Nirich melt-quenched ribbons containing Zr or Hf, the thermal stability was investigated by differential scanning calorimetry (DSC), transmission electron microscopy (TEM) and thermomagnetic measurements for the amorphous Zr-Fe, Zr-Co and Zr-Ni as well as the bcc-Ni(Zr) alloy ribbons. For the amorphous alloys, a general tendency is that both the crystallization temperature and the enthalpy of crystallization decreases in the sequence $Fe \rightarrow Co \rightarrow Ni$. A comparison of two a-ZroFeo1 ribbons prepared with different quenching rates revealed that for the lower quenching rate the activation energy and the crystallization temperature are slightly smaller due to the larger number of quenched-in nuclei. For the a-ZrqCoq1 alloy, the crystallization products were found to be fcc-Co + Zr₆Co₂₃ and although a single DSC peak only occurs, TEM studies indicated that the precipitation of Zr₆Co₂₃ preceeds the appearance of fcc-Co. For the Ni-based alloys, the phase transformation occurs at practically the same temperatures for both the amorphous and bcc states and the final phases are the same (fcc-Ni + ZrNi₅). The transformation temperatures determined from thermomagnetic measurements agreed well with the corresponding DSC data and the magnetization changes accompanying the phase transformation could be well interpreted on the basis of DSC and TEM results. The phase transformation sequences during thermal decomposition were investigated in more detail for the Ni-rich melt-quenched bodycentered cubic (bcc) and amorphous Ni-Zr alloys. A single DSC peak was observed for both the bcc and amorphous Ni91Zr9 alloys and a two-step process was indicated by DSC for the amorphous $Ni_{90}Zr_{10}$ alloy. In the bcc- $Ni_{91}Zr_{9}$ alloy which is actually a Ni(Zr) solid solution phase, the phase transformation starts with the precipitation of Ni5Zr crystallites followed, after a sufficient depletion of the matrix in Zr, by the subsequent transformation of the bcc-Ni(Zr) lattice to face-centered cubic (fcc) Ni. In the amorphous alloy of the same composition, the final products are fcc-Ni and Ni5Zr but at intermediate stages of the phase transformation, bcc-Ni(Zr) crystallites also appear. In the a-Ni₉₀Zr₁₀ alloy, the first DSC peak corresponds to the formation of the bcc-Ni(Zr) phase which then decomposes (second DSC peak) to the equilibrium phases fcc-Ni and Ni5Zr. Thus, in addition to the previous observation of the formation of the metastable bcc-Ni(Zr) phase by rapid quenching from the melt, here we have presented evidence that this phase can form also after partial crystallization of metallic glasses of appropriate chemical compositions.

Metallic multilayers. — Our previous structural study performed by conventional transmission electron microscopy (TEM) on electrodeposited Ni-Cu/Cu multilayers exhibiting giant magnetoresistance (GMR) has been extended by using atomic-resolution TEM. It could be established from these structural studies that (i) the layered structure found by conventional TEM to be flat and smooth shows an interface roughness spread over a few atomic monolayers; (ii) the atomic planes cross, in most cases, continuously the Ni-Cu/Cu interface, i.e., forming a coherent superlattice; (iii) the atomic planes exhibit a periodic distortion due to the unrelaxed strain induced by the lattice mismatch between the magnetic and non-magnetic constituent layers. Furthermore, the GMR of electrodeposited Ni₈₁Cu₁₉/Cu multilayers were studied also as a functon of the Cu layer thickness. For this purpose, electrodeposited Ni₈₁Cu₁₉/Cu

multilayers were produced from a sulfate bath by pulse-plating with $d_{Ni-Cu} = 3$ nm and with d_{Cu} varying from 0.5 to 3 nm and their in-plane magnetoresistance and magnetization were measured in magnetic fields up to 20 kOe at room temperature. The amplitude and width of the magnetoresistance curves varied systematically with Cu layer thickness, in each case exhibiting a GMR contribution as well. An oscillatory behaviour of the GMR was found with peaks at 1 and 2.5 nm Cu layer thicknesses and a similar oscillation could be revealed in the width as well. Around the main GMR peak, the magnetoresistance curve consisted of a sharply and a slowly saturating component, whereas for $d_{Cu} \ge 1.5$ nm, only the latter component survived.

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Grants

OTKA T015649	Giant magnetotransport phenomena in nanophase metals (I. Bakonyi, 1995-1998)
OTKA T016670	NMR relaxation and local properties in solids (K. Tompa, 1995- 1998)
OTKA T 022 124	Preparation and investigation of single-phase nanocrystalline metals (I Bakonyi, 1997-2000)
CNRS-HAS Joint re	esearch project No. 3064: Microstructure, magnetic properties and magnetoresistance of magnetic metallic multilayers and alloy films (I. Bakonyi, 1996-1997)

Publications

Articles

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Conference proceedings:

I.12. W. Schwarzacher^{*}, M. Alper^{*}, R. Hart^{*}, G. Nabiyouni^{*}, I. Bakonyi and E. Tóth-Kádár: Electrodeposited magnetic nanostructures. In: *Proc. of the Symposium P: "Electrochemical Synthesis and Modification of Materials" held at the Materials Research Society Fall Meeting* (Boston, Dec. 2-6, 1996) MRS Symp. Proc. Vol. **451**, pp.347-357 (1997)

J. METALLURGY AND MAGNETISM

<u>L.K. Varga</u>, J. Garaguly, P. Kamasa, G. Konczos, A. Lovas⁺, J. Pádár, L. Pogány, B. Varga⁺⁺, I. Varga⁺⁺

Study of soft magnetic nanocrystalline alloys. — The thermomagnetic study of soft magnetic nanocrystalline alloys has been continued. Formerly, we have investigated the T_c of bcc nanograins as a function of annealing by high heating rate magnetization measurements and have demonstrated their supersaturated state. This time, we have monitored the magnetic decoupling of the nanograins by initial permeability μ_i measurements and have demonstrated that at high temperatures but still below the T_c of nanograins, a superparamagnetic transition occurs for both types of nanocrystalline materials (Fe-Si-B based FINEMET and Fe-Zr-B based NANOPERM). The thermal dependence of the initial permeability around the T_c of the amorphous precursor reveals a huge Hopkinson peak as an indication of the preponderance of magnetization rotation over domain wall displacement magnetization process around the peak temperature. We have found, as a general rule, that the first peak of the μ_i thermogram (Hopkinson peak) shifts towards lower temperatures and broadens while its amplitude goes through a maximum. At the same time, the second, superparamagnetic peak shifts towards higher temperatures preserving its sharp form while its amplitude shows a maximum as a function of annealing. As a rule of thumb, the optimal annealing corresponds to the largest superparamagnetic transition peak. Tailoring for best soft magnetic properties includes both as high as possible magnetization and initial permeability. The latter condition can be achieved when the Hopkinson peak is around the working temperature. At present, none of the two types of material fulfills this condition: the maximum permeability for FINEMET is above while for NANOPERM it is below room temperature. To preserve the high permeability in a large temperature interval, a composite of differently annealed samples has been recommended.

Furthermore, to clarify some details of nanophase formation from FINEMET-type precursors, the thermomagnetic (TM) and calorimetric (DSC) data for alloys with different Nb contents have been compared. The main features of the DSC thermograms (shape, relative separation of the exothermic peaks) and thermomagnetic curves were interpreted in terms of the basic decomposition processes in Fe-B and Fe-B-Si glassy systems. The changes in magnetic losses and the induced anisotropy during heat treatment were compared for some FINEMET-type and Fe-Zr-based nanocrystalline alloys.

To improve our measurements on soft magnetic materials, a digital signal processing has been developed in cooperation with the Institute of Physics of the A. Mickiewicz University of Poznan. The new method is based on narrow band coherent digital phase sensitive detection (DPSD). The noise is reduced by using the Gabor transform. By the new method, the magnetic losses have been measured up to 100 kHz in nanocrystalline samples.

The distribution of elements in fungi. — The Hungarian Research Fund supported the ion distribution investigation in arbuscular micorrhizal fungi. The investigation ion distribution of Glomus spores gave new results for Ca, P and K as macroelements.

⁺ Also with the Technical University of Budapest

⁺⁺ Ph.D. student (Technical University of Budapest)

The effects of the environmental components as - water, soil - on the ion distribution were also investigated. The Zn content was found to be two order of magnitude higher in the fungi than in the soil.

Magnetic domain studies by SEM. — The domain structure in soft magnetic metallic glasses has been studied by Scanning Electron Microscopy (SEM) using type II magnetic contrast in the backscattered electron image. Fe₈₅B₁₅ and FINEMET type glassy ribbons were investigated in as-quenched state and after different heat treatments (with and without applied magnetic field). The magnetic domain structure inside the bulk material can also be analysed by taking backscattered electron images at three different accelerating voltages. The motion of magnetic domains under the influence of a periodic magnetic field has been filmed by using the stroboscopic imaging mode.

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Grants

OTKA T020891	Study	of	intracellular	element	distribution	in	soil
	microorganisms (L. Pogány, 1996-1999)						
GE-TUNGSRAM:	Contract for materials research by SEM (L. Pogány, 1997)						

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- J.5. É. Kisdi-Koszó^{*}, L.F. Kiss, L.K. Varga, P. Kamasa: Curie temperature measurement of metastable alloys using high heating rate. *Mater. Sci. Eng. A* 226-228, 689-692 (1997)
- J.6. L.K. Varga, A. Lovas, L. Pogány, L.F. Kiss, J. Balogh, T. Kemény: The role of nucleating element additives in the crystallization and soft magnetic properties of Fe-Zr-B based amorphous alloys. *Mater. Sci. Eng. A* 226-228, 740-744 (1997) (see also D.6.)
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- J.13. L.K. Varga D. Kaptás and T. Kemény: Soft magnetic nanocrystalline powders obtained by mechanical grinding. In: *Intern. Symposium on Mechanically alloyed and Nanocrystalline Materials ISMANAM97*, Barcelona (Spain), accepted for publication (see also D.26.)
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K. NON-DESTRUCTIVE EVALUATION

<u>F. Tóth</u>

Feasibility of corrosion detection in steel pipe using the magnetostrictive sensor technique. — Corrosion of insulated steel pipes is a serius problem commonly encountered in petrochemical, oil and electric power industries. To inspect these pipes cost-effectively, therefore, non-destructive evaluation techniques are needed that do not require removal lagging and interrupt operation.

In ferrous materials such as steel tubes and cables, mechanical or elastic wave can be transmitted and detected without direct physical contact, based on the phenomenon known as magnetostriction (Joule effect) and inverse magnetostriction (Villari effect). The Joule effect refers to a physical change in the dimensions due to magnetization and the Villari effect refers to a magnetic induction change due to mechanical strain and stress.

The use of elastic waves in material inspection offers various potential benefits, including inspection over long distances from a single sensor location, inspection of inaccessible areas and, in particular, the ability to transmit and detect these waves without direct physical contact.

Deterioration of the entire cross section of pipe or steel bridge strands (corrosion, internal or external defects) can be inspected simultaneously, thus providing fast and efficient testing and increasing the cost-effectiveness.

To determine the feasibility of inspecting pipes and boiler tubes using the magnetostrictive sensor approach, experimental setup and instrumentation is under construction. The pulse-echo technique is used in this experiment employing two separate sensors, one for transmitting and the other for receiving the mechanical waves. Each sensor produces steady DC magnetization to generate longitudinal wave modes only. The transmitting coil is excited by high frequency tone burst. The induced voltage in the receiving coil is amplified, bandpass filtered and displayed on an oscilloscope.

The developed instruments and method will be tested at the Hungarian nuclear power plant (Paksi Atomerõmû RT).

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

K.2. F. Tóth: Tárolótartály fenéklemez vizsgáló mérőrendszer (Tank Floor Tester, in Hungarian). *Anyagvizsgálók Lapja* **7**, 39-41 (1997)

L. NEUTRON SCATTERING IN CONDENSED MATTER

<u>L. Rosta</u>, L. Almásy, S. Borbély, L. Cser, T. Grósz, P. Jóvári, Gy. Káli, L. Kõszegi, L. Riecsánszky, Gy. Török

The neutron beam lines of the 10 MW Budapest Research Rector (BRR) were basically used to perform neutron scattering investigations of structural and dynamic properties of condensed matters, some special experiments, however, were performed at other neutron source facilities (ISIS, HMI Berlin, LLB Saclay). We operate at BRR a pinehole collimation type small angle scattering (SANS) instrument and a triple axis spectrometer (TAS) both installed on neutron guides. Another TAS instrument and a 4-circle materials test diffractometer are being installed on thermal neutron beams. A new reflectometer was recently installed on a neutron guide, we are sharing the construction and utilisation of this instrument.

The Neutron Physics Department on one hand operates the above experimental stations, on the other hand provides services for external users to perform experiments and exploit the obtained results. In 1997 nearly 50 experiments were completed by the local staff and in collaboration with national or foreign users coming from university, industrial or other research laboratories. In the followings a few examples of this research activity will be listed.

A series of measurements was performed and the first results reported on the investigation of the behaviour of acoustic phonons at the phase transformation from the dynamically to statically disordered network of hydrogen bonds in $Cs_5D_3(SO_4)$ (PCTS) crystals. Inelastic neutron scattering experiments at room temperature were performed on the triple axis spectrometer. The dispersion curve of the TA phonons along the $[00\xi]$ direction in a hexagonal phase was observed. The temperature dependencies of the TA and mixed phonon branches along [110] were studied.

A SANS study revealed the orientational stabilisation of the smectic structure by nonmesogenic polymer networks dispersed in a liquid crystal matrix. In the present experiment hydrophobic silica particles were dispersed in liquid crystal 8CB. The Bragg-reflections from smectic layers show that the alignment of the layers is perfect if the system is cooled down in a magnetic field. After annealing without magnetic field and cooling down to smectic A phase, the previous alignment of the liquid crystal recovers. The effect of temperature and the silica particle concentration dependence has been measured by recording the diffraction pattern from smectic layers.

The investigation of morphology of potassium containing bubbles in a series of doped tungsten wire samples by SANS experiments revealed that the shape of oriented ellipsoid particles - potassium bubbles - can be directly observed on the isointensity contour map measured by two-dimensional position sensitive detector. Samples of W wire, used as raw material for lamp filaments, at different stages of thermomechanical treatment were measured. Samples immediately after the wire drawing show strong anisotropy persisting to a smaller extent in samples after intermediate heat treatment and vanishing in the completely annealed samples. The results were interpreted in terms of a simple model with mixture of ellipsoid shaped and spherical dispersoid potassium particles.

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Grants

OTKA T 22486	Investigation of sintering processes using neutron scattering methods (T. Grósz, 1997-2000)
OTKA T 4490	Complex investigation of hydrophobic effects in aqueous solutions
OTKA T 16943	Decomposition of liquid crystal based binary systems (L. Rosta)
OTKA T 17016	Ordering phenomena in interface and surface thin layers (L.
	Cser)
AKP 96/2-406 2,2	Investigation of phase transitions in metastable systems (L.
	Cser, 1997-1998)
EU Network: WEN	NET Neutron scattering in molecular systems
EU PECO	Use of neutron source facilities at LLB Saclay

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Articles

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- L.2. G. Kádár^{*}, G. Káli, Cs. Dücsõ^{*}, É.B. Vázsonyi^{*}: Small angle neutron scattering in porous silicon. *Physica* B, **234-236**, 1014-1015, (1997)
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- L.4. S. Ansell^{*}, L. Cser, T. Grósz, G. Jancsó^{*}, P. Jóvári, A. Soper^{*}: Solute-solute correlation in aqueous solution of tetramethylurea. *Physica B*, **234-236**, 347-348 (1997)
- L.5. L. Almásy, L. Cser, I. Dézsi^{*}, G. Káli: Small angle neutron scattering (SANS) study of frozen solutions. *Physica* B, **234-236**, 82-83 (1997)
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Conference proceeding:

L.12. T. Grósz, P. Harmat^{*}, O. Horacsek^{*}, Gy. Káli, L. Rosta: SANS study of Potassium Filled Bubbles in Thermomechanically Treated Tungsten. In: *"Materials Research Using Cold Neutrons as Pulsed Neutron Sources"*, 25-26 August, ANL, Argonne, U.S.A, accepted for publication

M. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, S. Varró

Multiphoton-electron interaction processes in metals. — We verified experimentally those intense field QED predictions, according to which electronelectron, and electron-photon collision in metals strongly change the high order coherence properties of multiphoton processes. We demonstrated that depending on the ratio of the laser frequency value and the collision rate, respectively, the photoelectron emission extremely increased and at the same time, the multiharmonic light generation completely suppressed. These new phenomena which could not been observed at short wavelengths were demonstrated now by us with a long wavelength IR free electron laser. The effect may be controlled either by tuning the wavelength or by changing the metal temperature, which fact may furnish new possibilities for the practice in producing high current laser cathodes and tuneable high harmonic light sources.

High order autocorrelation of ultrashort pulses with multiphoton detection. — After dividing and delaying in a Michelson-interferometer, we directed our picosecond laser pulses onto a metal cathode inducing here multiphoton electron emission. We determined the very high (5th) order intensity correlation and fringe-resolved correlation functions with extremely high (512) contrast value. This procedure presents a new possibility to study theoretically the ultrafast high order multiphoton processes, and at the same time, furnishes a new method for the ultrashort time metrology, which independent of the wavelength and the phase-matching.

We also elaborated a new theoretical model for studying sophisticated phaseinfluences for the fringe resolved autocorrelation in the case of chirped laser pulses.

Theoretical studies on interaction of strong laser fields with matter. — We have theoretically studied the interaction of high intensity laser fields with matter. In particular we have proved that the effect of target dressing in free-free transitions of an electron in a bichromatic laser field plays a crucial role in small angle scattering. We have constructed a new model to describe multiphoton photoeffect and harmonic generation at metal surfaces, and explained the outcome of experiments carried out at our institute on this subject. Concerning quantum optics, we have introduced a generalization of the Moyal-equation of a quantized mode of the electromagnetic radiation, and proved that trough gauge transformation one can easily construct Wigner functions of non-classical states of that mode.

Laser driven electron acceleration and X-ray generation. — We elaborated general and summarizing theoretical studies on the laser acceleration of electrons to GeV energies on generation of terawatt X-ray pulses using multiphoton interaction processes.

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Grants:

OTKA I/7 T16014	Experimental and theoretical investigation of new fundamental physical processes (laser-matter interactions) induced by laser beams of superintense $(10^{15} - 10^{20} \text{ W/cm}^2)$ laser systems. (Gy. Farkas, 1995–1998)
BALATON 6/95	High harmonic generation in the interaction of laser pulses with surfaces: investigation of the phenomenon in the infrared at high laser intensities. (Gy. Farkas, 1995–1997)

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N. LASER PHYSICS

<u>M. Jánossy</u>, G. Báno, T.J. Bereczki, L. Csillag, Z. Donkó, Sz. Fórizs, Á. Hoffmann, Z. Gy. Horváth, Zs. Lenkefi, P. Mezei, K. Rózsa, L. Szalai, K. Szõcs, Zs. Szentirmay

Gas lasers and glow discharges in (segmented) hollow cathodes. — Our research in this topic covers investigations of cathode-sputtered gas – metal ion lasers and computer modeling and experimental studies of low pressure glow discharges. We developed a hybrid model of a hollow cathode discharge where the particle (Monte Carlo) treatment of fast electrons is combined with the fluid description of slow electrons and buffer gas ions. The Monte Carlo treatment of fast electrons provides a fully kinetic description - necessary because of the highly non-equilibrium nature of the electrons' motion in the cathode region of glow discharges. Our model provides a fully self-consistent solution of the continuity and momentum balance equations of electrons and ions, and the Poisson equation. Further steps were made towards the optimization of the discharge arrangements to enhance the small signal gain of metal ion laser transitions. The effect of the cathode to anode surface ratio and of different electrode configurations on the characteristics of the He-Cu 780.8 nm laser operating in a segmented hollow cathode discharge was experimentally investigated. The results of the measurements were analyzed by applying Monte Carlo simulation of the fast electrons' motion in the discharge. The simulations provided electron energy distributions in the discharge and information about details of the fast electrons' behavior at different electrode configurations.

He–Zn hollow cathode laser. — In a He–Zn discharge it was observed that addition of Ne stops laser oscillation at the 492.4 nm Zn ion line and increases significantly the spontaneous intensity at the 210.0 nm Zn ion line, which originates from the lower level of the laser transition. Based on a rate equation model the cross-section of the Ne ion – Zn atom charge transfer collisions populating the lower laser level was determined. The cross-section was found to be 3.5×10^{-15} cm², which is in a good agreement with the experimental value 2.3×10^{-15} cm² published earlier in the literature.

Electrolyte cathode atmospheric glow discharge (ELCAD). — The electrolyte cathode atmospheric glow discharge is a new optical emission source for direct analysis of heavy metal content of water. The occurrence of atomic metal lines in the emitted spectrum of the ELCAD requires a matrix concentration of 0.03-0.1 M of a strong acid or its salt. Investigating the effect of different matrix anions presenting in the solution on the intensity of atomic metal lines, a significant increase of the intensity was found in case of the chloride anions compared with that obtained using nitrate and sulphate anions. This effect was even more emphasized, when the appropriate acids were applied.

A further enhancement of the metal line intensities could be observed, when the HCl was used in the solution phase and simoultaneously elementary chlorine was mixed into the atmospheric air up to 6-10 volumetric percent. This double effect was especially high for the resonant atomic line of the Cu, Ni and Pb. At higher chlorine/air ratio in the gas phase, the W-anode tip was destroyed by chemical burning.

The application of volatile organic chlorine compounds (carbon-tetrachloride and chloroform) in the gas phase, however, without any acidification of the solution, caused also an enhancement of the metal line intensities.

The experimental results can be attributed to the ion - ion recombination process taking place between the positive metal ions produced by the cathode sputtering and the negative chlorine ions. Since the rate of this recombination is higher with orders of magnitude than that of the positive metal ion - electron recombination , the density of excitable neutral metal atoms increases in the negative glow, and it causes the enhancement of atomic metal line intensities.

Determination of optical constants of thin films with multichannel ATR reflectometry. Optical parameters of metallic and non-metallic thin films (complex dielectric function and the thickness) can be determined by measurement of the attenuated total reflection (ATR) of light. In this method the first layer should be a surface-plasmon-carrying metal film as e.g. silver or gold, while the 100-200 Å thick adlayers could be both metallic or non-metallic.

The basic unit of our newly developed multichannel reflectometer is a conventional ATR reflectometer, working in the Kretschmann geometry. The light source is a white lamp unit and the analysis of the reflected beam is performed using an OMA-4 multichannel optical analyzer. This instrument makes possible the determination of the angular distribution of reflectance of thin film samples in the 400-900 nm wavelength region in one cycle. The first measurements were made on C_{60} films of 10-50 nm thickness.

Research on multidimensional lasers. — A preliminary experimental setup was constructed to realize 2-dimensional planar laser radiation in gas discharges, but the observed gain values were below the expectations. The theoretical investigation of "natural plasmas" i.e. the behaviour of stars, from the point of view of possible natural, star laser processes were started. According to our results amplified spontaneous emission can occur in stars in a natural way just because of the existence of the gravitational field.

In the field of photodinamic diagnose research we have determined the relationship between the 5- ALA concentration in the culturing medium and the quantity of the induced endogenous porphyrins, as well as the time dependent accumulation of fluorescent porphyrins during the incubation time of cells.

In connection with the evaluation of complicated infrared spectra of organic compounds, computer simulations have shown the benefits of neural network data evaluation compared to classical statistical methods.

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Grants:

OTKA-T-14909 OTKA-F-15502	Lasers in hollow cathode discharges (K. Rózsa, 1995-1998) Basic processes of glow discharge in the cathode region (Z. Donkó, 1995-1998)
OTKA T-017293	Multidimensional lasers (Z. Gy Horváth; 1996-1998)
OTKA T-014850	Electrolyte cathode atmospheric glow discharge (P. Mezei, 1995-1998)
OTKA T-016075	Electromagnetic modes of metal/dielectric interfaces (N. Kroó, 1995-1998)
OTKA T-020089	Optical parameters of fullerene films (Zs. Szentirmay, 1996- 1999)
OTKA T-022074	Investigation of metal fullerene films with laser reflectometry (Á. Hoffmann, 1997-2000)

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- N.4. Z. Donkó, L. Szalai, K. Rózsa, M. Ulbel^{*}, M.Pöckl^{*}: High gain ultraviolet Cu-II laser in a segmented hollow cathode discharge. *IEEE J. Quantum Electronics*, accepted for publication.
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- N.9. Á. Hoffmann, N. Kroó, Z. Lenkefi, Z. Szentirmay: The influence of the surface roughness of the optical parameters of gold films. In: *Kvantumelektronika*'97, *Proc. of the 3rd National Conference on Quantum Electronics*. (30. October, 1997. Budapest), Ed.: S. Varró (KFKI, Budapest, 1997), P56 (in Hungarian)
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- N.13. P. Mezei: Gas lasers operating in near infrared, visible and ultraviolet region.
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O. LASER APPLICATION

<u>I. Kertész,</u> A. Czitrovszky, P. Jani, A. Kiss, M. Koós, Gy. Messing, Said H.S. Moustafa, A. Nagy, B. Plósz, I. Pócsik

Solid state laser development. — A Q switched Nd-YAG laser was built for high quality material processing in the frame of a TD&QM EU Phare Programme. The system is capable for continuous and pulsed operation up to 300-500 W average output power. Our piezo driven Fabry-Perot unit served as an output mirror (with adjustable reflection) or as output mirror-Q switch (with reflection jump from zero to optimum) at 0-100 kHz repetition rates.

Optical measurement technique. — A new version of the PC controlled liquid-borne particle counter (LQB-1-200-L-T) was developed in which a new method was used for determination of the size distribution and concentration of the particles suspended in liquids having wide viscosity range. This method is based on the simultaneous measurement of the pulse-height and pulse-duration of the photoelectric impulses which corresponds to the passing of the particles to be tested through the illuminated volume and evaluation of these signal by two independent multi-channel analysers. The possibility of the determination of the form-factor of the measured particles is analysed.

A new portable battery operated note-book PC-controlled airborne particle counter PAPC-03-2 was developed for determination of the size distribution and concentration of sub-micron- and micron-range particles in air and in gases at low and high concentrations. The device has a number of benefits in comparison with the previous version and was successfully exhibited at Hannover Messe-1997.

New results were obtained with the previously developed high resolution sampling laser interferometer at Machine Tool Department of the Miskolc University. The mechanical transient phenomena studied by this device provide the determination and analysis of the displacement and vibration parameters of the mechanical system with high resolution and precision.

The experimental set-up for investigation of the high temperature aerosols release in simulated LWR accident - in air ingress experiment - is under further development.

A new high time resolution electronic system was elaborated for investigation of the statistical properties of the non-classical entangled state of the light.

A book entitled "Trends in Laser Development, Application and Technologies" was edited, and different chapters were written in it.

Amorphous thin layers.—The investigations have been focused on the diamond-like amorphous carbon (a-C:H). In connection with atomic scale structure investigations the vibrational properties have been studied with Raman and resonant Raman scattering methods. Macroscopic properties related to the electronic states near to band edges and to the localised states deep in the forbidden gap have been investigated by dc electrical conductivity and photoluminescence behaviour. Our experimental work was motivated by the border line problems of the a-C:H research i.e. what sort of cluster structures are formed by the sp² coordinated carbon atoms; how the transport properties of a-C:H differing strongly from other tetrahedrally coordinated amorphous materials can be explained; furthermore, what is the mechanism of the effective room temperature photoluminescence.

The Raman spectra of a-C:H samples shows a close similarity to the spectrum of the graphite, and its interpretation was also based on it. Our preliminary results suggested, that there are assignation problems in the Raman spectrum of the amorphous carbon, and graphite. We have carried out a systematic resonant Raman investigation of graphite crystals, and showed, that one of the two most intensive characteristic graphite lines (D line) is not a simple Raman line, it shifts with excitation energy. It is consequence of an electron excitation, which is followed by an emission of a phonon of the same volume element of the reciprocal space, where the electron transition took place. The Raman shift corresponds to the frequency of the phonon, far from the zone centre. Comparison of the Stokes and anti-Stokes spectrum proved this idea.

Non-Arrhenius temperature dependence of dc conductivity was observed in different sp^2 hybridised carbon containing a-C:H samples, the actual activation energy (E_{act.}) increased with increasing temperature. Different mechanisms were suggested to interpret this behaviour, like variable range hopping and multi-phonon tunnelling. Our investigation on a systematic sample series showed that this behaviour is in close connection with the width of the tail states. The broad distribution of tail states, the lack of mobility edges, might result in T^{-1/4} behaviour even above room temperature. That dependence was observed in the samples containing sp^2 carbons in smaller concentration. The samples with larger concentration of these carbon atoms in which the tail states show a more band-like character, the temperature dependence of conductivity begins to exhibit Arrhenius behaviour.

A crucial question of luminescence mechanism in a-C:H was answered by extending the measurement of the photoluminescence excitation spectra to the UV range. We proved, that the photoluminescence efficiency decreases, when the excitation energy approaches the diamond gap energy. We have clearly demonstrated, that the light emitting transitions are related to the π electron transitions.

Grants

OTKA T 017371	Diamond-like amorphous carbon; atomic bonds, nanostructure and macroscopic properties (M. Koós, 1995-1997)
OTKA 20202	Development of fundamental experiments with squeezed light
	(A. Czitrovszky, 1996-1999)
AKP 96/2-615 2.2	Development of high time resolution and high quantum
	efficiency photodetection system (A. Czitrovszky, 1996-1999)
OMFB-Technoorg	SZFKI 1018-95 Development of a new liquid-bortne particle
	counter (A. Czitrovszky, 1996-1997)
OMFB 47-0980	Development of portable airborne particle counter (P. Jani, 1996-1997)

Publications

Articles

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- O.3 I. Pócsik, M. Koós, S.H. Moustafa, J.A. Andor^{*}, O. Berkesi^{*} and M. Hundhausen^{*}: Comparative Raman Studies of Hydrogenated Amorphous Carbon Films using Infrared and Visible Laser Excitations. *Microchim. Acta [Suppl.]* 14, 755-56 (1997).
- O.4 M.S. Iovu^{*}, E.P. Colomeico^{*}, M. Koós and I. Pócsik: Conductivity and Photoconductivity in a-C:H/p-Si Heterojunctions. *Romanian Journal of Optoelectronics* **5**, 29-32 (1997).
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- O.9. I. Pócsik, M. Koós, M. Hundhausen^{*} and L. Ley^{*}: Excitation Energy Dependent Raman and Photoluminescence Spectra of Hydrogenated Amorphous Carbon. In: *Expert Rewievs on Amorphous Carbon*, Ed. by S.R.S. Silva, Word Scientific, Singapore, accepted for publication.

Books and book chapters

- O.10. I. Kertész: Solid State Lasers. In: *Trends in Laser Development, Application and Techniques*, ed. by A. Czitrovszky, I. Kertész; Technorg-Linda Ltd. Co. Budapest, 1997, pp. 41-45.
- O.11. A. Czitrovszky: Laser light scattering methods and their applicatons in micron and submicron particle measurements. In: *Trends in Laser Development*, *Application and Techniques*, ed. by A. Czitrovszky, I. Kertész; Technorg-Linda Ltd. Co. Budapest, 1997, pp.105-127
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Optoelectronics; NATO ASI Series Edited by A. Andriesh and M. Bertolotti, Kluwer Academic Publishers, Dordrecht (1997) pp. 361-378.

P. OPTICAL THIN FILMS

K. Ferencz, P. Apai, R. Szipõcs

Optical thin film structures in femtosecond laser systems. — Continuing our research started in 1993, dispersive dielectric mirrors were developed for different femtosecond laser systems such as low-loss chirped mirrors for mode-locked Cr:LiSGaF, Cr:LiSAF lasers, for broadly tunable cw and modelocked Ti:sapphire lasers and IR KTP based parametric oscillators. The Ti:sapphire oscillators built at the Technical University of Vienna, Austria and at ETH Zürich, Switzerland, utilize our chirped mirrors for intra- and extracavity dispersion compensation, and deliver the shortest pulses (7.5 fs) ever obtained directly from a laser oscillator. Sub-20-fs pulses were obtained from Cr:LiSGaF and Cr:LiSAF lasers capable of direct diode pumping. 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 Wien, coherent X-ray emission was detected from a laser induced He plasma in the water window.

White light interferometry for dispersion measurement on laser mirrors, laser active materials and other cavity elements. — Group delay dispersion (GDD) vs. frequency functions of several laser active materials such as Cr:LiSAF, Cr:LiSGaF, Cr:LiCAF, Ti:sapphire, Yb:glass, Nd:GGG etc. and a photorefractive material (BaTiO₃) were measured by using interference in the frequency domain.

High efficiency phase conjugation of broadband laser pulses in BaTiO3. — Phase conjugation of spectrally broad femtosecond laser pulses was demonstrated by spectrally dispersing the pulses in a photorefractive BaTiO3 crystal using our mode-locked, mirror-dispersion controlled Ti:S laser oscillator in cooperation with ICTP Trieste, Italy. Cavity mirrors of the Ti:S oscillator were designed to exhibit minimum losses to allow the laser operate around 700 nm.

Other developments on optical coatings. — Low loss dielectric mirrors have been developed for hollow cathode copper and gold lasers. The mirrors have been successfully tested at the Department of Laser Physics.

Our work on optical waveguides deposited on optical gratings are still in progress for optical sensors used for medical applications. We investigated the effect of surface relief grating on the morphology and waveguiding properties of the deposited dielectric layers.

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Grants

OTKA T-020568 Dispersive dielectric mirrors for femtosecond laser systems (R. Szipõcs, 1996-1998).

- OTKA CW-015285 Dispersion measurement on optical thin film structures and other optical element using white light interferometry (R. Szipõcs, 1996-1998).
- OMFB Project A 53/96 Mirror-dispersion controlled, diode pumped, modelocked solid state lasers (R. Szipõcs, 1996-1998)

Publications

Articles

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EDUCATION

Graduate and postgraduate courses, 1997

- Statistical physics (F. Iglói, JATE³)
- Computational Physics (F. Iglói, JATE)
- Thermodynamics and statistical physics (F. Iglói, JATE)
- Advanced solid state physics II. (J. Sólyom, ELTE⁴)
- Mathematics of the Heisenberg and Hubbard modells (A. Sütő, ELTE)
- Solid state physics II. (A. Virosztek, BME)
- Superconductivity (I. Tüttõ, BME)
- Advanced solid state physics I. (I. Tüttõ, ELTE)
- Semiconductors (I. Tüttõ, BME)
- Completely integrable many body systems (F. Woynarovich, ELTE)
- Completely integrable many body systems (F. Woynarovich, KLTE)
- Theory of Magnetism I. (P. Fazekas, BME)
- Theory of Magnetism II. (P. Fazekas, BME)
- Solid state physics (I. Vincze, ELTE)
- Solid state research I (I. Vincze, ELTE)
- Modern experimental methods in solid state physics (G. Faigel ELTE, BME)
- Experimental methods in materials science (G. Faigel, K. Kamarás BME)
- Spectroscopy and structure (K. Kamarás BME)
- Physics of liquid crystals and polymers (Á. Buka, ELTE)
- Physics for Life Sciences Majors: Electricity and Magnetism (G. Kriza, UCLA)
- Group Theory in Solid State Physics (G. Kriza, BME)
- Beyond the Crystalline State (A. Jákli, BME)
- Advanced material technologies (G. Konczos, BME)
- From metals to ceramics (A. Lovas, BME)
- NMR Spectroscopy (K. Tompa, BME)
- Nanophase metals: Electrical transport and magnetic properties (I. Bakonyi, ELTE)

³JATE: Attila József University, Szeged

⁴ELTE: Loránd Eötvös University, Budapest,

Laboratory practice and seminars

- Laboratory for solid state physics, Preparation and crystallization of metallic glasses (I. Vincze, ELTE)
- Solid State Physics (L. Gránásy, BME)
- Infrared spectroscopy (K. Kamarás, ELTE)
- Solid State Physics Seminar (G. Kriza, BME)
- Advanced Solid State Physics Laboratory (G. Mihály and G. Kriza, BME, ELTE)
- Experiments on liquid crystals (Á. Buka, ELTE)
- Basic experimental physics (A. Jákli, BME)
- NMR spectroscopy (K. Tompa, ELTE-BME)
- Laser optical laboratory (L. Szalai, BME)
- Medical application of lasers (Z. Gy. Horváth ; HIETE, Medical Laser Center)
- Measurements on an experimental He-Ne laser (T. J. Bereczki, K. Szőcs, BME)
- Seminars on biophysics for medical students (K. Szőcs, SOTE)
- General physics, seminar (Sz. Fórizs, BME)

Diploma works

- P. Varga (BME): Resistivity and Hall-effect in superconducting cuprates (consultant: A. Virosztek)
- I. Farkas (ELTE): Approach to magnetic saturation in soft magnetic systems (consultant: I. Vincze)
- A. Király (ELTE): Physical Properties of columnar liquid crystals (consultant: A. Jákli)
- B. Alföldi (ELTE): Multicomponent spin-spin relaxation and consequences in tomography (consultant: K. Tompa)
- B. Varga (BME): Study of the mechanism of the am-nc transformation.

Ph. D. students

- T. Tóth Katona: Pattern formation at the interfaces of liquid crystal phases (Supervisor: Á. Buka)
- T. Börzsönyi: Oscillatory shear induced instabilities in nematic liquid crystals (Supervisor: Á. Buka)
- E. Szabó, Synthesis and properties of ferroelectric liquid crystals (Supervisor: K. Fodor-Csorba)
- M. Bokor: NMR relaxation in Fe and Zn ionic crystals (Supervisor: K. Tompa)
- T. Marek: NMR spectra in Fe and Zn ionic crystals (Supervisor: K. Tompa)

- J. Garaguly: Mechanism of hydrogen absorption and desorption (Supervisor: A. Lovas)
- I. Varga: Magnetic domain contrast studies and image processing by SEM (Supervisor: L. Pogány)
- B. Varga: Investigation of rapidly quenched nanocrystalline systems (Supervisor: A. Lovas)
- Gy. Káli: Investigations of dynamical behaviour of macromolecular solutions and suspensions by the use of neutron small angle scattering. (Supervisor: L. Rosta)
- P. Jóvári: Structure investigation of solutions using neutron scattering methods and quantum chemical approaches. (Supervisor: L. Cser)
- L. Almásy: Investigation of metastable systems by neutron scattering (Supervisor: L. Cser)
- L. Szalai: Au laser in segmented hollow cathode discharge (Supervisors: K. Rózsa and Z. Donkó)
- G. Bánó: Cathode sputtered Zn laser (Supervisors: K. Rózsa and Z. Donkó)
- K. Szõcs: Fluorescence imaging (Supervisor: Z. Gy. Horváth)
- T. J. Bereczki: Tunable laser simulator (Supervisor: Z. Gy. Horváth)
- Sz. Fórizs: Application of neurochips in optics (Supervisor: Z. Gy. Horváth)
- Said H.S. Moustafa: Amorphous carbon thin layers, structure and macroscopic physical properties (supervisor: Margit Koós)

Dissertations

- K. Kamarás: Electron and phonon contributions in the infrared spectra of high Tc materials (Doctor of Physical Science, Hungarian Academy of Sciences)
- S. Pekker: Solid state chemical properties of conjugated polymers and fullerenes (Doctor of Chemical Science, Hungarian Academy of Sciences)
- G. Kriza: Collective Electronic excitations of spin-density waves (Doctor of Physical Science, Hungarian Academy of Sciences)
- K. Rózsa: UV lasers in high efficiency hollow cathode discharges (Doctor of Physical Science, Hungarian Academy of Sciences)
- K. Fodor-Csorba: Synthesis of liquid crystals and C₆₀ chlatrates (Ph. D., ELTE TTK)

Awards

- N. Kroó, Alexander von Humboldt Research Award
- L. Bata, Main award for Physics of the Hungarian Academy of Sciences
- L. Szalay, Award for young Scientists of the Hungarian Academy of Sciences
- E. Szabó, 2nd prize on the National Scientific Conference of Students, Pécs
- I. Farkas, 1st prize, Student's Scientific Work (TDK), ELTE

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